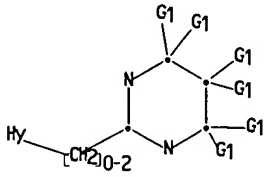
C:\STNEXP4\QUERIES\10009477 (rce).str

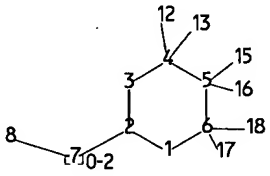
Ak@2

Cb@1



2@2

19@1

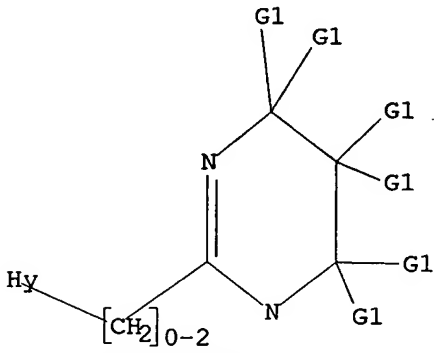


chain nodes :
7 8 12 13 15 16 17 18 19 20
ring nodes :
1 2 3 4 5 6
chain bonds :
2-7 4-12 4-13 5-15 5-16 6-17 6-18 7-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
4-12 4-13 5-15 5-16 6-17 6-18 7-8
exact bonds :
1-2 1-6 2-3 2-7 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,Cl,Br,F,I,Hy,[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 12:CLASS 13:CLASS
15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 20:CLASS
Generic attributes :
8:
Saturation : Unsaturated
19:
Saturation : Unsaturated
20:
Saturation : Saturated

```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L1    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L2    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10009477 (rce).str

L3      STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4   QUE L3 AND L1 NOT L2

=> d 14
L4 HAS NO ANSWERS
L1              SCR 1839
L2              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L3              STR

Ak 2




Cb 1
```

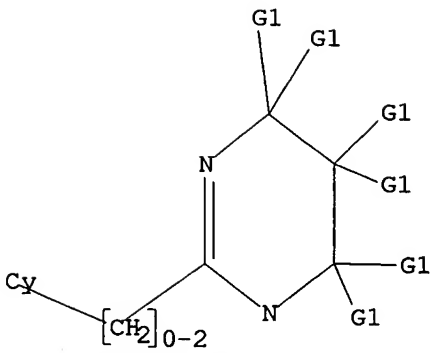



```
G1 H,Cl,Br,F,I,Hy,[@1],[@2]


Structure attributes must be viewed using STN Express query preparation.
L4              QUE  L3 AND L1 NOT L2
```

```
=> s l4 sss sam
SAMPLE SEARCH INITIATED 21:20:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   8720 TO ITERATE

 11.5% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       168806 TO   179994
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L3 AND L1 NOT L2

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L6    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L7    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10009477 (rce).str

L8      STRUCTURE UPLOADED

=> que L8 AND L6 NOT L7

L9   QUE L8 AND L6 NOT L7

=> d l9
L9 HAS NO ANSWERS
L6              SCR 1839
L7              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L8              STR
```

Ak 2

Cb 1



G1 H,Cl,Br,F,I,Hy,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.
L9 QUE L8 AND L6 NOT L7

=> s l9 sss sam
SAMPLE SEARCH INITIATED 21:21:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8720 TO ITERATE

11.5% PROCESSED 1000 ITERATIONS 15 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 168806 TO 179994
PROJECTED ANSWERS: 1930 TO 3302

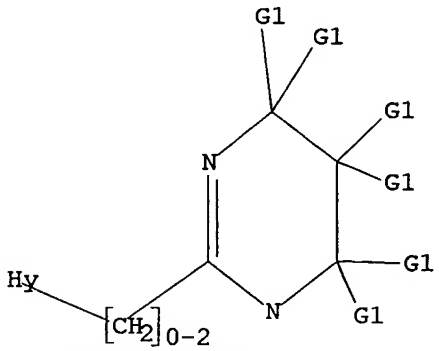
L10 15 SEA SSS SAM L8 AND L6 NOT L7

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):....Testing the current file....
screen

'SCREEN' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

```
=> screen 1839

L11    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L12    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10009477 (rce).str

L13      STRUCTURE UPLOADED

=> que L13 AND L11 NOT L12

L14  QUE L13 AND L11 NOT L12

=> d l14
L14 HAS NO ANSWERS
L11              SCR 1839
L12              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L13              STR


Ak 2




Cb 1
```




```
G1 H,Cl,Br,F,I,Hy,[@1],[@2]


Structure attributes must be viewed using STN Express query preparation.
L14              QUE  L13 AND L11 NOT L12


=> s l14 sss sam
```

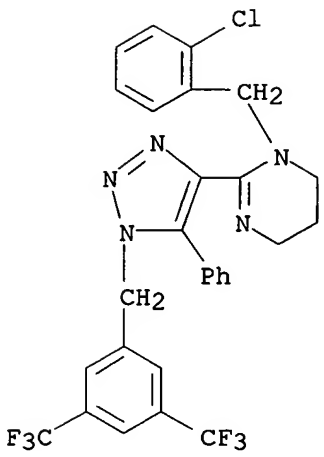
```
SAMPLE SEARCH INITIATED 21:22:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   8720 TO ITERATE

 11.5% PROCESSED    1000 ITERATIONS                                 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       168806 TO   179994
PROJECTED ANSWERS:               0 TO        0

L15           0 SEA SSS SAM L13 AND L11 NOT L12

=> s l14 sss ful
FULL SEARCH INITIATED 21:22:55 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 174632 TO ITERATE

100.0% PROCESSED  174632 ITERATIONS                             105 ANSWERS
SEARCH TIME: 00.00.03

L16         105 SEA SSS FUL L13 AND L11 NOT L12

=> s l16
L17          39 L16

=> d l17 1-39 bib,ab,hitstr
```

L17 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:875262 CAPLUS
DN 139:364937
TI Preparation of triazole derivatives as tachykinin receptor antagonists
IN Amegadzie, Albert Kudzovi; Gardinier, Kevin Matthew; Hembre, Erik James; Hong, Jian Eric; Jungheim, Louis Nickolaus; Muehl, Brian Stephen; Remick, David Michael; Robertson, Michael Alan; Savin, Kenneth Allen
PA Eli Lilly and Company, USA
SO PCT Int. Appl., 188 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003091226	A1	20031106	WO 2003-US10681	20030422

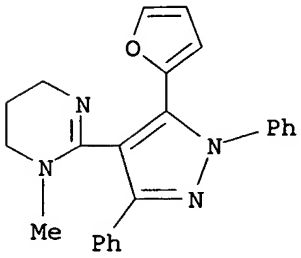
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2002-376121P P 20020426
OS MARPAT 139:364937
AB The title compds. [I; D = alkanediyl; R1 = (un)substituted Ph; R4 = 2-chlorobenzoyl(or benzyl) substituted (hetero)aryl, etc.; R5 = H, halo, alkyl, etc.], useful as inhibitors of the NK-1 subtype of tachykinin receptors, were prepd. Thus, reacting (2-bromopyridin-3-yl)(2-chlorophenyl)methanone with 1-[3,5-bis(trifluoromethyl)benzyl]-5-methyl-4-tributylstannyl-1H-[1,2,3]triazole in the presence of PdCl2(PPh3)2 in DMF afforded 54% II. Pharmaceutical compn. comprising the compd. I is claimed.
IT **622372-68-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of triazole derivs. as tachykinin receptor antagonists)
RN 622372-68-3 CAPLUS
CN Pyrimidine, 2-[1-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-phenyl-1H-1,2,3-triazol-4-yl]-1-[(2-chlorophenyl)methyl]-1,4,5,6-tetrahydro- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

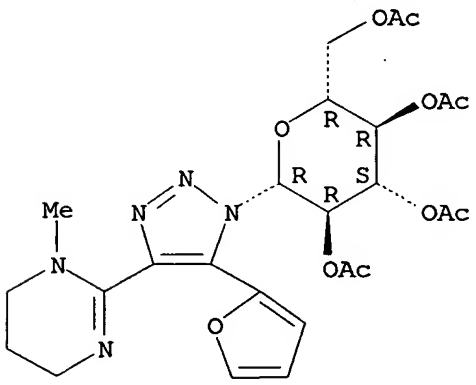
L17 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:855864 CAPLUS
DN 139:214344
TI Product class 1: pyrazoles
AU Stanovnik, B.; Svete, J.
CS Faculty of Chemistry and Chemical Technology, Division of Organic Chemistry, Ljubljana, 61000, Slovenia
SO Science of Synthesis (2002), 12, 15-225
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review. Methods for prepg. pyrazoles are reviewed including cyclization, ring transformation, aromatization and substituent modifications.
IT **251940-14-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(review of prepn. of pyrazoles via cyclization, ring transformation, aromatization and substituent modifications)
RN 251940-14-4 CAPLUS
CN Pyrimidine, 2-[5-(2-furanyl)-1,3-diphenyl-1H-pyrazol-4-yl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)



RE.CNT 909 THERE ARE 909 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

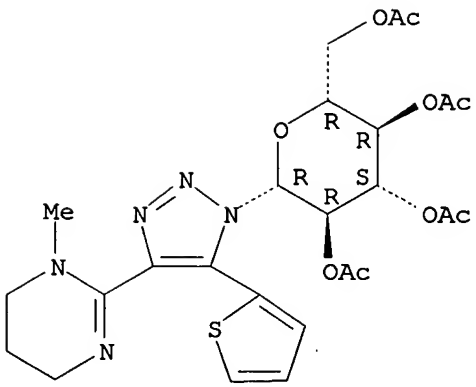
L17 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:331495 CAPLUS
DN 137:140703
TI The reaction of heteroaryl-substituted heterocyclic ketene aminals with 2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl azide
AU Yang, Qiang; Li, Zhan-Jiang; Chen, Xiao-Min; Huang, Zhi-Tang
CS Center for Molecular Sciences, Institute of Chemistry, The Chinese Academy of Sciences, Beijing, 100080, Peop. Rep. China
SO Heteroatom Chemistry (2002), 13(3), 242-247
CODEN: HETCE8; ISSN: 1042-7163
PB John Wiley & Sons, Inc.
DT Journal
LA English
OS CASREACT 137:140703
AB The cyclocondensation reaction of heteroaryl-substituted heterocyclic ketene aminals with 2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl azide was investigated and a series of potential bioactive compds., 1-glucopyranosyl-4-heterocyclic-5-heteroaryl-1,2,3-triazoles, were obtained in good yields. Both the reaction rate and the yield were strongly affected by the heteroaryl and heterocyclic groups. In order to improve their water soly., the deprotection of 1-glucopyranosyl-4-heterocyclic-5-heteroaryl-1,2,3-triazole, e.g. I, was carried out.
IT **444995-30-6P 444995-31-7P 444995-32-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cyclocondensation of heteroaryl-substituted heterocyclic ketene aminals with 2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl azide in prepn. of 1-glucopyranosyl-4-heterocyclic-5-heteroaryl-1,2,3-triazole)
RN 444995-30-6 CAPLUS
CN Pyrimidine, 2-[5-(2-furanyl)-1-(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)-1H-1,2,3-triazol-4-yl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



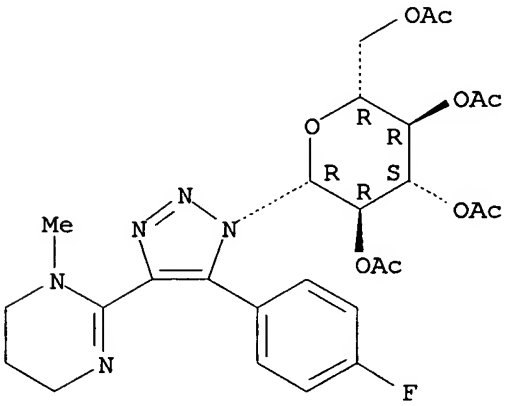
RN 444995-31-7 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[1-(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)-5-(2-thienyl)-1H-1,2,3-triazol-4-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



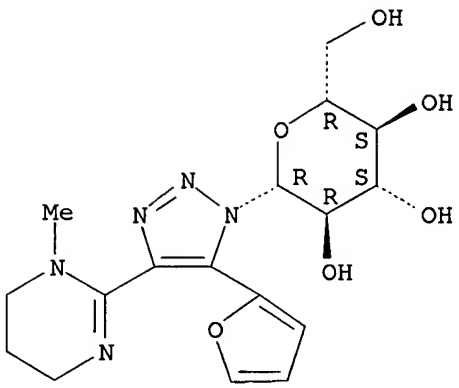
RN 444995-32-8 CAPLUS
CN Pyrimidine, 2-[5-(4-fluorophenyl)-1-(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)-1H-1,2,3-triazol-4-yl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



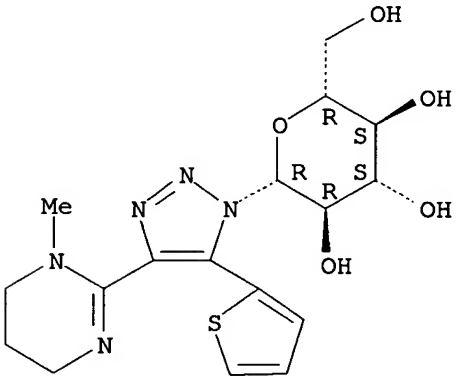
IT **444995-38-4P 444995-39-5P 444995-40-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclocondensation of heteroaryl-substituted heterocyclic ketene aminals with 2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl azide in prepn. of 1-glucopyranosyl-4-heterocyclic-5-heteroaryl-1,2,3-triazole)
RN 444995-38-4 CAPLUS
CN Pyrimidine, 2-[5-(2-furanyl)-1-.beta.-D-glucopyranosyl-1H-1,2,3-triazol-4-yl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



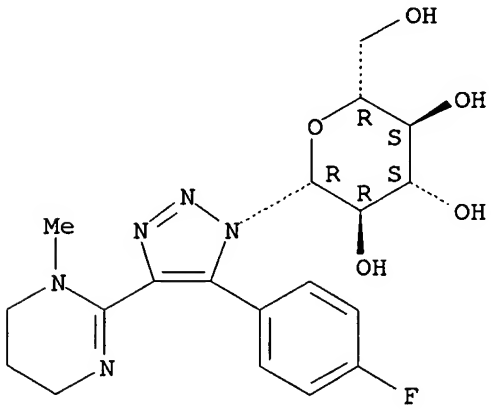
RN 444995-39-5 CAPLUS
CN Pyrimidine, 2-[1-.beta.-D-glucopyranosyl-5-(2-thienyl)-1H-1,2,3-triazol-4-yl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 444995-40-8 CAPLUS
CN Pyrimidine, 2-[5-(4-fluorophenyl)-1-.beta.-D-glucopyranosyl-1H-1,2,3-triazol-4-yl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)

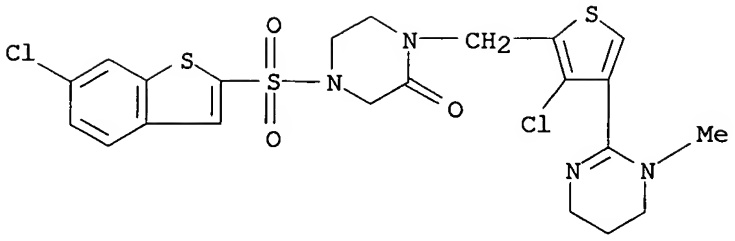
Absolute stereochemistry.



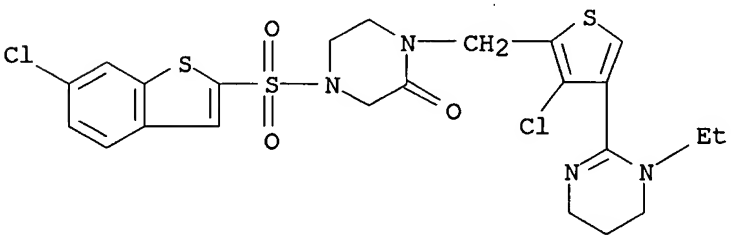
L17 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:256255 CAPLUS
DN 136:279479
TI Preparation of piperazin-2-one amides as inhibitors of factor Xa
IN Zhu, Bing-yan; Su, Ting; Li, Wenhao; Goldman, Erick A.; Zhang, Penglie; Jia, Zhaozhong Jon; Scarborough, Robert M.
PA Cor Therapeutics, Inc., USA
SO PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002026734	A1	20020404	WO 2001-US30313	20011001
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002011280	A5	20020408	AU 2002-11280	20011001
	EP 1322643	A1	20030702	EP 2001-979304	20011001
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	US 2000-236393P	P	20000929		
	WO 2001-US30313	W	20011001		

OS MARPAT 136:279479
AB The title compds. [I or II; A = MeNHC(:NH), 1-methylimidazol-2-yl; PrNMeC(:NH), etc. R = H, alkyl, cycloalkyl, etc.; Q = III-VII; R1 = H, halo, alkyl, etc.; J1 = (un)substituted Ph, pyridyl, pyrimidinyl, furyl, thienyl; J2 = (un)substituted 2-naphthyl, 2-benzothienyl, etc.; n = 0-2; m = 1-2; p = 0-1], having activity against mammalian factor Xa (no data given), and useful in vitro or in vivo for preventing or treating conditions in mammals characterized by undesired thrombosis, were prepd. E.g., a multi-step synthesis of VIII was given.
IT **406492-98-6P 406492-99-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of piperazin-2-one amides as inhibitors of factor Xa)
RN 406492-98-6 CAPLUS
CN Piperazinone, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-1-[[3-chloro-4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-2-thienyl]methyl]- (9CI) (CA INDEX NAME)



RN 406492-99-7 CAPLUS
CN Piperazinone, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-1-[[3-chloro-4-(1-ethyl-1,4,5,6-tetrahydro-2-pyrimidinyl)-2-thienyl]methyl]- (9CI) (CA INDEX NAME)



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:256243 CAPLUS
DN 136:294851
TI Preparation of piperazine (hetero)aryl ketones and sulfones as factor Xa inhibitors for treatment of thrombosis or coagulation disorders
IN Zhu, Bing-Yan; Jia, Zhaozhong Jon; Zhang, Penglie; Huang, Wenrong; Wu, Yanhong; Zuckett, Jingmei Fan; Goldman, Erik A.; Wang, Lingyan; Song, Yonghong; Scarborough, Robert M.
PA Cor Therapeutics, Inc., USA
SO PCT Int. Appl., 128 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002026720	A2	20020404	WO 2001-US30315	20011001
WO 2002026720	A3	20021031		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1322610	A2	20030702	EP 2001-975505	20011001

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

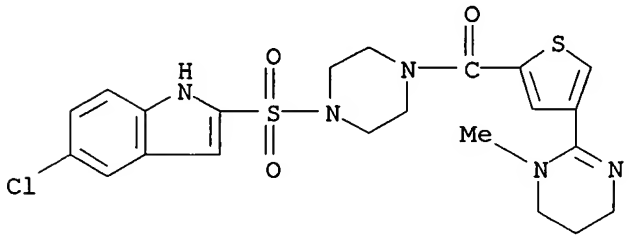
PRAI US 2000-236161P	P	20000929	
WO 2001-US30315	W	20011001	

OS MARPAT 136:294851
AB Title compds. I [wherein A = (un)substituted imidazolinyl, tetrahydropyrimidinyl, tetrahydro-1H-1,3-diazepinyl, imidamido(alkyl), guanidinyl, amino(alkyl), ammoniomethyl, Ph, pyridinyl, etc.; Q = (un)substituted phenylene, pyrimidinediyl, pyridinediyl, pyrazinediyl, pyrroldiyl, furandiyl, thiophenediyl, piperidinediyl, or pyrrolidinediyl; V = CH2 or CO; G = CO or SO2; J = (un)substituted naphthyl, (iso)quinolinyl, quinazolinyl, indolyl, benzothiophenyl, benzofuranyl, benzimidazolyl, benzothiazolyl, benzoxazolyl, etc.; R1 and R2 = independently H, alkyl, hydroxyalkyl, aminoalkyl, cyanoalkyl, carboxyalkyl, alkoxycarbonylalkyl, or carbamoylalkyl; and pharmaceutically acceptable isomers, salts, hydrates, solvates, and prodrugs thereof] were prepd. For example, 1-Boc-5-chloro-2-indolylsulfonyl chloride was coupled with 1-Boc-piperazine in DCM in the presence of pyridine to give the sulfonamide (95%). Deprotection using HCl gas (99%), followed by acylation with 4-cyanobenzoyl chloride in pyridine in the presence of DMAP (73%) and treatment with HCl and dimethylamine, afforded II. I are highly selective inhibitors of factor Xa and are useful for the treatment of diseases characterized by undesired thrombosis or coagulation disorders (no data).
IT **406716-11-8P 406716-32-3P 406716-47-0P 406716-64-1P 406716-81-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(factor Xa inhibitor; prepn. of piperazine (hetero)aryl ketones and

sulfones as factor Xa inhibitors for treatment of thrombosis or coagulation disorders)

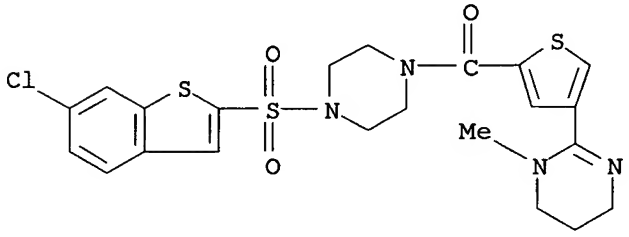
RN 406716-11-8 CAPLUS

CN Piperazine, 1-[(5-chloro-1H-indol-2-yl)sulfonyl]-4-[[4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)



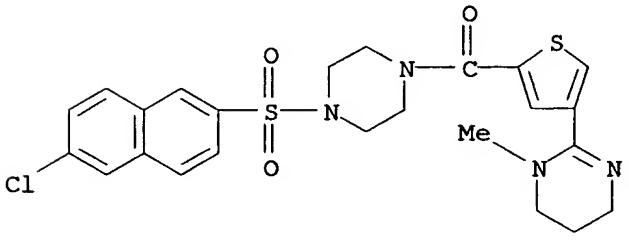
RN 406716-32-3 CAPLUS

CN Piperazine, 1-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-4-[[4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)



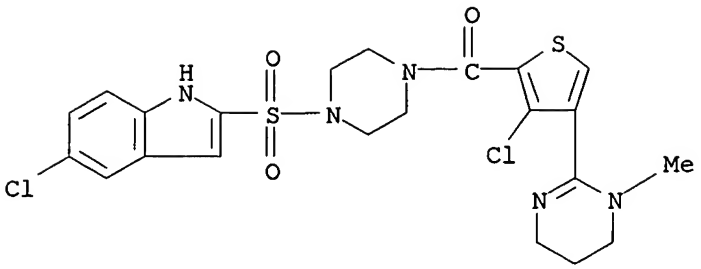
RN 406716-47-0 CAPLUS

CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[[4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)

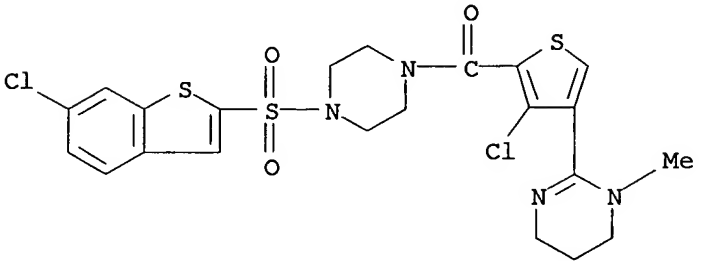


RN 406716-64-1 CAPLUS

CN Piperazine, 1-[(5-chloro-1H-indol-2-yl)sulfonyl]-4-[[3-chloro-4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)



RN 406716-81-2 CAPLUS
CN Piperazine, 1-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-4-[[3-chloro-4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-2-thienyl]carbonyl]- (9CI) (CA INDEX NAME)



L17 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2001:793434 CAPLUS
DN 135:339275
TI Cyclic amidines, nicotinic acetylcholine .alpha.4.beta.2 receptor activators containing them, and pharmaceuticals
IN Imoto, Masahiro; Iwanami, Tatsuya; Akabane, Minako; Tani, Yoshihiro
PA Suntory, Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

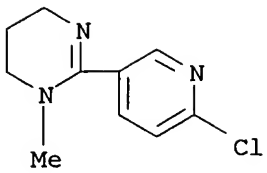
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001302643	A2	20011031	JP 2000-120976	20000421
	WO 2001081334	A2	20011101	WO 2001-JP3378	20010420
	WO 2001081334	A3	20020808		
	W: AU, CA, CN, KR, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	AU 2001048799	A5	20011107	AU 2001-48799	20010420
	EP 1280793	A2	20030205	EP 2001-921932	20010420
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
	US 2003100769	A1	20030529	US 2001-9477	20011211
PRAI	JP 2000-120976	A	20000421		
	WO 2001-JP3378	W	20010420		

Appl. JP/PCT.

OS MARPAT 135:339275
AB The activators, useful for treatment of brain function disorders, contain cyclic amidines I [A1, A2 = H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocyclyl; X = (un)substituted C2H4, (un)substituted CH:CH, (un)substituted (CH2)3, (un)substituted CH2CH2NH] or their salts. Trimethylenediamine was cyclocondensed with Et (6-chloro-3-pyridyl)acetate and treated with fumaric acid to give I fumarate (A1 = H, A2 = 6-chloro-3-pyridylmethyl, X = CH:CH), which showed affinity with rat nicotinic acetylcholine .alpha.4.beta.2 receptor with Ki of 29 nM, vs. 1.6 nM, for nicotine. Pharmaceutical formulations contg. I are given.
IT **371121-82-3P 371121-93-6P 371122-39-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyclic amidines as nicotinic acetylcholine .alpha.4.beta.2 receptor activators)
RN 371121-82-3 CAPLUS
CN Pyrimidine, 2-(6-chloro-3-pyridinyl)-1,4,5,6-tetrahydro-1-methyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

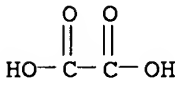
CM 1

CRN 371121-81-2
CMF C10 H12 Cl N3



CM 2

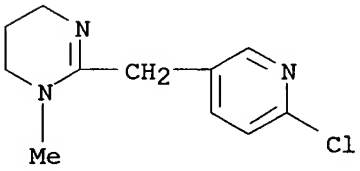
CRN 144-62-7
CMF C2 H2 O4



RN 371121-93-6 CAPLUS
CN Pyrimidine, 2-[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro-1-methyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

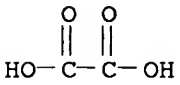
CM 1

CRN 371121-92-5
CMF C11 H14 Cl N3



CM 2

CRN 144-62-7
CMF C2 H2 O4

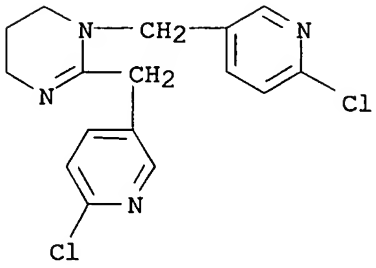


RN 371122-39-3 CAPLUS
CN Pyrimidine, 1,2-bis[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-38-2

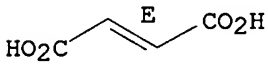
CMF C16 H16 Cl2 N4



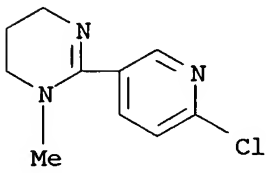
CM 2

CRN 110-17-8
CMF C4 H4 O4

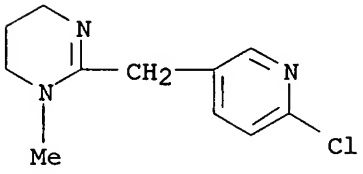
Double bond geometry as shown.



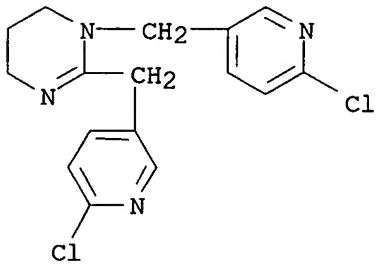
IT **371121-81-2 371121-92-5 371122-38-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of cyclic amidines as nicotinic acetylcholine .alpha.4.beta.2 receptor activators)
RN 371121-81-2 CAPLUS
CN Pyrimidine, 2-(6-chloro-3-pyridinyl)-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)



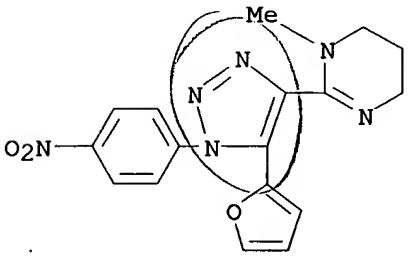
RN 371121-92-5 CAPLUS
CN Pyrimidine, 2-[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)



RN 371122-38-2 CAPLUS
CN Pyrimidine, 1,2-bis[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro- (9CI) (CA INDEX NAME)



L17 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:707783 CAPLUS
DN 134:4908
TI The reaction of aroyl-substituted heterocyclic ketene aminals with aryl azides
AU Liu, Bo; Wang, Mei-Xiang; Wang, Li-Ben; Huang, Zhi-Tang
CS Center for Molecular Sciences, Institute of Chemistry, The Chinese Academy of Sciences, Beijing, 100080, Peop. Rep. China
SO Heteroatom Chemistry (2000), 11(6), 387-391
CODEN: HETCE8; ISSN: 1042-7163
PB John Wiley & Sons, Inc.
DT Journal
LA English
OS CASREACT 134:4908
AB Aroyl-substituted heterocyclic ketene aminals reacted with p-chlorophenyl azide to give polysubstituted 1,2,3-triazoles as well as fused heterocycles. The aroyl-substituted heterocyclic ketene aminals reacted with p-nitrophenyl azide much faster, and polysubstituted 1,2,3-triazoles were obtained as sole products.
IT **308360-64-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of aroyl-substituted heterocyclic ketene aminals with aryl azides)
RN 308360-64-7 CAPLUS
CN Pyrimidine, 2-[5-(2-furanyl)-1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl]-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:707168 CAPLUS
DN 133:266871
TI Novel 4-substituted quinoline derivatives as GABA receptor ligands
IN Yuan, Jun; Hutchison, Alan
PA Neurogen Corp., USA
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA English

Same as #7

FAN.CNT 2

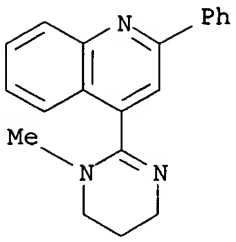
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000058313	A1	20001005	WO 2000-US8196	20000328
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6413982	B1	20020702	US 2000-536922	20000328
	US 2002198232	A1	20021226	US 2002-140693	20020507
	US 6624175	B2	20030923		
PRAI	US 1999-126926P	P	19990329		
	US 2000-536922	A1	20000328		

OS MARPAT 133:266871

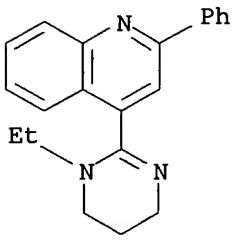
AB The title compds. I [R1 = H, halo, OH, C1-6alkyl, -O(C1-6alkyl), NO2, CN, SO2NH2 (un)substituted amine, etc.; R2, R3 = (un)substituted-alkyl, -cycloalkyl, -alkenyl, -alkynyl {substituents selected from OH, oxo, F, (un)substituted amines, (un)substituted aryl, etc.}, (un)substituted aryl, (un)substituted arylamine, (un)substituted alkyl amine, N-contg. heterocycle, etc.; R4 = H, halo, OH, C1-8alkyl, -O(C1-8alkyl), NO2, CN, SO2NH2 (un)substituted amine, etc.; R5 = (un)substituted imidazolyl, (un)substituted fused (cycloalkyl)-, (heterocyclic)-imidazolyl] are prepd. and disclosed as ligands with high affinity for binding to GABAA receptors (no data). Thus, II was prepd. via condensation of 2-phenyl-4-quinolinecarboxylate with (S)-2-(aminomethyl)pyrrolidine. Also disclosed are pharmaceutical compns. comprising these compds., and methods of treating patients suffering from certain central nervous system and peripheral diseases or disorders with these pharmaceutical compns. This invention also relates to the use of such compds. in combination with one or more other CNS agents to potentiate the effects of the other CNS agents. A method for prepg. radiolabeled derivs. of I is described allowing for the use of I as probes for the localization of GABAA receptors.

IT **298195-94-5P 298195-95-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; prepn of 4-substituted quinoline derivs. as GABA receptor ligands)

RN 298195-94-5 CAPLUS
CN Quinoline, 2-phenyl-4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)



RN 298195-95-6 CAPLUS
CN Quinoline, 4-(1-ethyl-1,4,5,6-tetrahydro-2-pyrimidinyl)-2-phenyl- (9CI) (CA INDEX NAME)



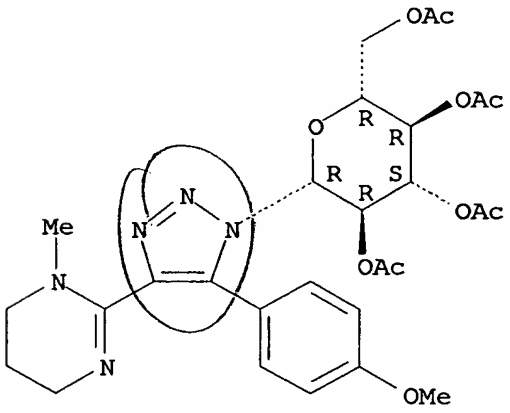
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:163014 CAPLUS
DN 132:180820
TI Synthesis of heterocyclic radical, sugar radical polysubstituted triazoles
IN Huang, Zhitang; Li, Zhanjiang; Chen, Xiaomin; Ren, Zhongshu; Wang, Meixiang; Li, Bo; Wang, Liben; Wang, Heting
PA Chemical Inst., Chinese Academy of Sciences, Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 9 pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CN 1188771	A	19980729	CN 1996-107062	19960712
	CN 1063183	B	20010314		
PRAI	CN 1996-107062		19960712		

OS CASREACT 132:180820; MARPAT 132:180820
AB Title compds. [I; X = C6H5, 4-CH3C6H4, 4-ClC6H4, 4-CH3OC6H4, 4-BrC6H4; R1 = H, CH3; R = CH3, C2H5, Ac, C6H5CO, C6H5CH2; n = 3, 4; saccharide = Oxygen contg. ring = D-pyranogalactosyl, D-pyranoglucosyl, D-pyranomannitosyl, L-pyranorhamnosyl, D-pyranoarabinosyl] are prepd. as antitumor, antiviral agent by substituting 1,2,3-triazoles with diazo-substituted-saccharide (mole ratio 2-6:2.5-6.5) in aprotic solvent at 10-100.degree. for 2-15 h. The title compd. II was prepd.
IT **259546-58-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of triazoles as antitumor agents)
RN 259546-58-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-2-[5-(4-methoxyphenyl)-1-(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)-1H-1,2,3-triazol-4-yl]-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

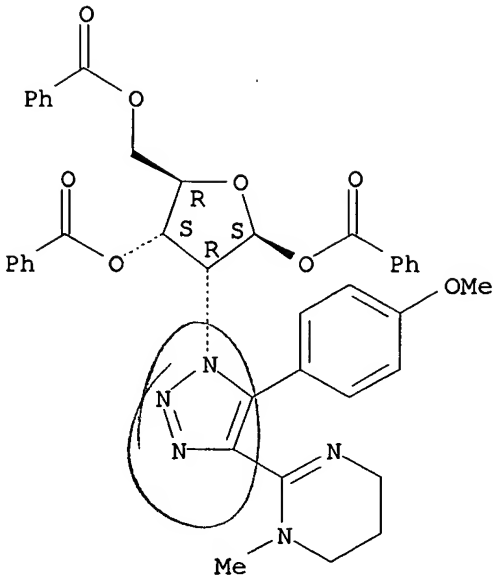


L17 ANSWER 13 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:304289 CAPLUS
DN 130:312018
TI Synthesis of heterocyclic ribosyl polysubstituted triazole compound
IN Huang, Zhitang; Li, Zhanjiang; Ren, Zhongxu; Chen, Xiaomin; Liu, Bo; Wang, Meixiang; Wang, Liben; Wang, Heting
PA Inst. of Chemistry, Chinese Academy of Sciences, Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 8 pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI CN 1170727	A	19980121	CN 1996-107065	19960712
PRAI CN 1996-107065		19960712		

OS MARPAT 130:312018
AB Title compds. [I; W is (CH2)m (m = 2,3,4); X is C6H5, 4-MeC6H4, 4-MeOC6H4, 4-ClC6H4, Ar, etc.; R1 = H, CH3; R2 = CH3, C6H5; R3 = Q, OR2; R4 = H, OR2, Q; R5 = H, OR2, Q], and stereoisomers are prepd. by dissolving heterocyclic ketene amine in non-protonic solvent (selected from THF, dioxane, and methylene dichloride), dripping non- protonic soln. contg. 3-7 mol triazo compd. I (R2 = CH3, C6H5; R3 = N3, OR2; R4 = H, OR2, N3; R5 = H, OR2, N3) in the system, reacting at 10-100.degree. for 2-20 h, removing solvent by reduced pressure distn., extg. product, and drying. Thus, I (X = 4-MeOC6H4, W = (CH2)3; R1 = H; R3 = Q; R4 = OCOPh; R5 = OCOPh) were prepd. from I (R3 = N3; R4, R5, R2 as above) and 4-MeOC6H4COCH2CH(NH)2(CH2)3.
IT **223498-23-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of heterocyclic ribosyl polysubstituted triazoles)
RN 223498-23-5 CAPLUS
CN .beta.-D-Ribofuranose, 2-deoxy-2-[5-(4-methoxyphenyl)-4-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-1H-1,2,3-triazol-1-yl]-, 1,3,5-tribenzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.


O
Ph
O
O
R
S
S
R
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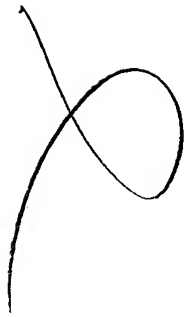
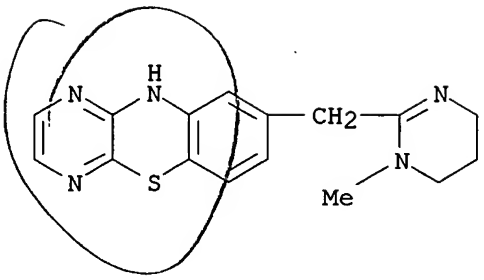
O
Ph
O
Ph
OMe
N
N
N
N
Me



L17 ANSWER 14 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:126254 CAPLUS
DN 128:204878
TI Preparation of pyrazinobenzothiazine derivatives and analogs for the treatment of inflammation and autoimmune diseases
IN Kaneko, Toshihiko; Clark, Richard; Ohi, Norihito; Ozaki, Fumihiro; Kawahara, Tetsuya; Kamada, Atsushi; Okano, Kazuo; Yokohama, Hiromitsu; Muramoto, Kenzo; Arai, Tohru; Ohkuro, Masayoshi; Takenaka, Osamu; Sonoda, Jiro
PA Eisai Co., Ltd., Japan; Kaneko, Toshihiko; Clark, Richard; Ohi, Norihito; Ozaki, Fumihiro; Kawahara, Tetsuya; Kamada, Atsushi; Okano, Kazuo; Yokohama, Hiromitsu; et al.
SO PCT Int. Appl., 1344 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

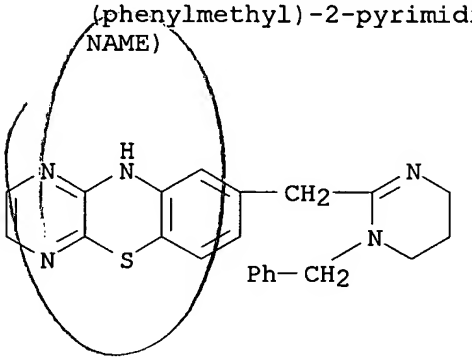
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9806720	A1	19980219	WO 1997-JP2787	19970808
	W: AU, CA, CN, HU, JP, KR, MX, NO, NZ, RU, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9737849	A1	19980306	AU 1997-37849	19970808
	ZA 9707103	A	19990208	ZA 1997-7103	19970808
	EP 934941	A1	19990811	EP 1997-934750	19970808
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	US 6518423	B1	20030211	US 1999-230852	19990405
PRAI	JP 1996-210344	A	19960809		
	WO 1997-JP2787	W	19970808		

OS MARPAT 128:204878
AB The title compds. I [R1 to R3 are the same or different and each represents hydrogen, optionally substituted lower alkyl, optionally substituted cycloalkyl, etc., provided that when R1 to R3 are all optionally substituted lower alkyl groups, they do not simultaneously represent Me groups; R represents hydrogen, lower alkyl, etc.; E represents N, C, etc.; Z represents O, S, SO, SO2, etc.; and the ring G represents an optionally substituted heteroaryl ring having at least one nitrogen atom] are prepd. I are useful in the treatment and prevention of inflammatory immunol. diseases, autoimmune diseases, rheumatism, collagen disease, asthma, nephritis, ischemic reflow disorders, psoriasis, atopic dermatitis or rejection reactions following organ transplantation. The compd. (syn)-[3-(10H-pyrazino[2,3-b][1,4]benzothiazin-8-ylmethyl)-3-azabicyclo[3.3.1]nona-9-yl]acetic acid (II) at 10 mg/kg orally gave 65% inhibition of carrageenin-induced inflammation in rats. II in vitro showed IC50 of 2.3 .mu.M against the expression of ICAM-1.
IT **203659-23-8P 203659-24-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrazinobenzothiazine derivs. and analogs for treatment of inflammation and autoimmune diseases)
RN 203659-23-8 CAPLUS
CN 1H-Pyrazino[2,3-b][1,4]benzothiazine, 8-[(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

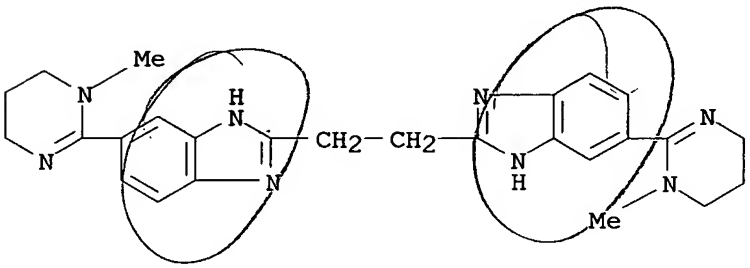
RN 203659-24-9 CAPLUS
CN 1H-Pyrazino[2,3-b][1,4]benzothiazine, 8-[[1,4,5,6-tetrahydro-1-(phenylmethyl)-2-pyrimidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 15 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1993:517175 CAPLUS
DN 119:117175
TI Structure, DNA minor groove binding, and base pair specificity of alkyl- and aryl-linked bis(amidinobenzimidazoles) and bis(amidinoindoles)
AU Fairley, Terri A.; Tidwell, Richard R.; Donkor, Isaac; Naiman, Noreen A.; Ohemeng, Kwasi A.; Lombardy, Richard J.; Bentley, James A.; Cory, Michael
CS Div. Org. Chem., Burroughs Wellcome Co., Research Triangle Park, USA
SO Journal of Medicinal Chemistry (1993), 36(12), 1746-53
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB A series of bis(amidinobenzimidazoles), e.g. I [X = (CH2)n, phenylene; n = 1-6], and bis(amidinoindoles), e.g. II (n = 3-6), with varied linking chains connecting the arom. groups and various modifications to the basic amidino groups have been prepd. The calf thymus (CT) DNA and nucleic acid homopolymer [poly(dA).poly(dT), poly(dA-dT)-poly-(dA-dT), and poly(dG-dC).poly(dG-dC)] binding properties of these compds. have been studied by thermal denaturation (.DELTA.Tm) and viscosity. The compds. show a greater affinity for poly(dA).poly(dT) and poly(dA-dT).poly(dA-dT) than for poly(dG-dC).poly(dG-dC). Viscometric (dA).poly(dT) and poly(dA-dT)-poly(dA-dT) than for poly(dG-dC).poly(dG-dC). Viscometric titrns. indicate that the compds. do not bind by intercalation. Mol. modeling studies and the biophys. data suggest that the mols. bind to the minor groove of CT DNA and homopolymers. Anal. of the shape of the mols. is consistent with this mode of nucleic acid binding. Compds. with an even no. of methylenes connecting the benzimidazole rings have a higher affinity for DNA than those with an odd no. of methylenes. Mol. modeling calcns. that det. the radius of curvature of four defined groups in the mol. show that the shape of the mol., as a function of chain length, affects the strength of nucleic acid binding. Electronic effects from cationic substituents as well as hydrogen bonding from the imidazole nitrogens also contribute to the nucleic acid affinity. The bis(amidinoindoles) show no structurally assocd. differential in nucleic acid base pair specificity or affinity.
IT **148344-19-8**
RL: PROC (Process)
(nucleic acid binding of)
RN 148344-19-8 CAPLUS
CN 1H-Benzimidazole, 2,2'-(1,2-ethanediyl)bis[5-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 16 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1988:529067 CAPLUS
DN 109:129067
TI Preparation of tetracyclic, fused-ring 1,4-diazepines as platelet-activating factor (PAF) antagonists
IN Weber, Karl Heinz; Harreus, Albrecht; Stransky, Werner; Walther, Gerhard; Casals, Stenzel Jorge; Muacevic, Gojko; Heuer, Hubert; Bechtel, Wolf Dietrich
PA Boehringer Ingelheim K.-G., Fed. Rep. Ger.
SO Ger. Offen., 68 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3724031	A1	19880128	DE 1987-3724031	19870721
	EP 254245	A1	19880127	EP 1987-110443	19870718
	EP 254245	B1	19940928		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	ES 2061452	T3	19941216	ES 1987-110443	19870718
	FI 8703180	A	19880123	FI 1987-3180	19870720
	PL 153970	B1	19910628	PL 1987-266884	19870720
	PL 157209	B1	19920529	PL 1987-287349	19870720
	DK 8703797	A	19880123	DK 1987-3797	19870721
	NO 8703041	A	19880125	NO 1987-3041	19870721
	NO 166942	B	19910610		
	NO 166942	C	19910918		
	JP 63033382	A2	19880213	JP 1987-182121	19870721
	JP 08005895	B4	19960124		
	ZA 8705333	A	19890329	ZA 1987-5333	19870721
	HU 50830	A2	19900328	HU 1987-3355	19870721
	HU 203354	B	19910729		
	DD 281389	A5	19900808	DD 1987-305190	19870721
	CS 274456	B2	19910411	CS 1987-5508	19870721
	CS 277445	B6	19930317	CS 1989-1930	19870721
	CS 277446	B6	19930317	CS 1989-1931	19870721
	AU 8776015	A1	19880128	AU 1987-76015	19870722
	AU 609408	B2	19910502		
	CA 1338287	A1	19960430	CA 1987-542748	19870722
	CZ 284052	B6	19980812	CZ 1989-2206	19890410
	SU 1738089	A3	19920530	SU 1989-4614791	19890817
	US 5532233	A	19960702	US 1994-302578	19940908
PRAI	DE 1986-3624647		19860722		
	US 1987-76515		19870722		
	US 1987-88758		19870824		
	US 1989-352527		19890516		
	US 1990-538582		19900614		
	US 1991-724654		19910702		
	US 1992-942556		19920909		
	US 1993-61392		19930513		

OS CASREACT 109:129067; MARPAT 109:129067
AB The title compds. [I; R1 = H, cycloalkyl, halo, (un)substituted alkyl, alkoxy; R2 = H, halo, cyano, CHO, OH, etherified or esterified OH, alkylthio, (un)modified CO2H, amino, benzimidazolyl, (un)substituted 5-, 6-, or 7-membered heterocyclyl; R3 = pyridyl, (un)substituted Ph; R4 = H, alkyl, alkanoyl; R5 = H; R4R5 = bond; X, Y = R6C, N; R6 = R1, alkoxycarbonyl; Z = bond, C1-6 alkylene; A = fused, unsatd.,

(un)substituted 5-, 6-, or 7-membered ring] and their stereoisomers and physiol. acceptable salts were prepd. as PAF antagonists. Cyclopentathienotriazolodiazepinecarboxylate II (R7 = EtO) was prepd. in 7 steps, starting with cyclocondensation of Et 3-oxocyclopentanecarboxylate with 2-ClC6H4COCH2CN. The ester was sapond. to give II (R7 = OH) which was treated with morpholine and 1,1'-carbonyldiimidazole to give morpholide II (R7 = morpholine) (III). III inhibited blood platelet aggregation with an IC50 of 0.3 .mu.M and, in the benzodiazepine receptor binding test, had an IC50 of 3600 .times. 10-9 M. In the same tests triazolam had an IC50 of 9 .mu.M and 1.4 .times. 10-9 M, resp. III is thus expected to have little CNS activity.

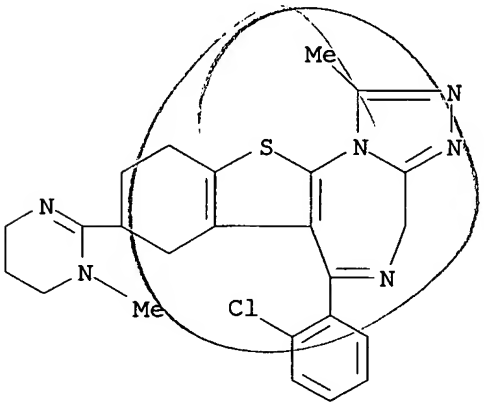
IT **114777-01-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

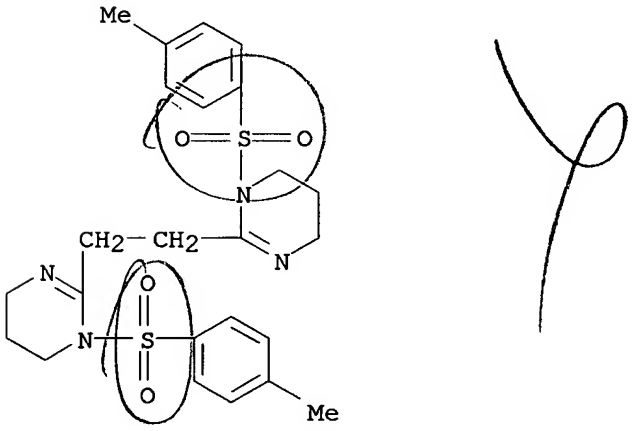
(prepn. of, as platelet-activating factor antagonist)

RN 114777-01-4 CAPLUS

CN 4H-[1]Benzothieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine, 6-(2-chlorophenyl)-7,8,9,10-tetrahydro-1-methyl-8-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 18 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1981:496272 CAPLUS
DN 95:96272
TI Regioselective carbonyl amination using diisobutylaluminum hydride
AU Yamamoto, Hisashi; Maruoka, Keiji
CS Dep. Chem., Univ. Hawaii, Honolulu, HI, 96822, USA
SO Journal of the American Chemical Society (1981), 103(14), 4186-94
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
AB A selective, and mild approach to N-alkylation of polyamines is demonstrated, which involves the novel reductive cleavage of the C-N bond in cyclic amidines by (Me2CHCH2)2AlH. This method provides a new entry to a wide variety of N-alkylated polyamines and interesting macrocyclic polyamines hitherto accessible only by lengthy or complicated synthesis.
IT **78707-11-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and methanolysis of)
RN 78707-11-6 CAPLUS
CN Pyrimidine, 2,2'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro-1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



L17 ANSWER 19 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1981:103366 CAPLUS
DN 94:103366
TI Urea and amido compounds
IN Marxer, Adrian
PA Ciba-Geigy A.-G., Switz.
SO S. African, 34 pp.
CODEN: SFXXAB
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ZA 7901062	A	19800326	ZA 1979-1062	19790307
	CA 1125759	A1	19820615	CA 1979-321545	19790215
	US 4292429	A	19810929	US 1979-14661	19790223
	FI 7900740	A	19790909	FI 1979-740	19790305
	FI 70708	B	19860626		
	FI 70708	C	19861006		
	EP 4561	A2	19791017	EP 1979-100647	19790305
	EP 4561	B1	19811104		
	EP 4561	A3	19791114		
	R: BE, CH, DE, FR, GB, IT, LU, NL, SE				
	CS 244656	B2	19860814	CS 1979-1460	19790305
	ES 478342	A1	19790516	ES 1979-478342	19790306
	DD 142336	C	19800618	DD 1979-211405	19790306
	PL 116762	B1	19810630	PL 1979-213924	19790306
	PL 123150	B1	19820930	PL 1979-221681	19790306
	IL 56797	A1	19820930	IL 1979-56797	19790306
	DK 7900952	A	19790909	DK 1979-952	19790307
	NO 7900765	A	19790911	NO 1979-765	19790307
	NO 152606	B	19850715		
	NO 152606	C	19851023		
	AU 7944900	A1	19790913	AU 1979-44900	19790307
	AU 531006	B2	19830804		
	AT 7901710	A	19810315	AT 1979-1710	19790307
	AT 364375	B	19811012		
	SU 845779	A3	19810707	SU 1979-2733999	19790307
	HU 25271	O	19830628	HU 1979-CI1920	19790307
	HU 182940	B	19840328		
	JP 54125668	A2	19790929	JP 1979-26245	19790308
	JP 62009109	B4	19870226		
	SU 923367	A3	19820423	SU 1980-2872253	19800118
	AT 8003951	A	19810515	AT 1980-3951	19800730
	AT 365179	B	19811228		
	US 4420619	A	19831213	US 1981-247427	19810325
	CS 244700	B2	19860814	CS 1984-8407	19841105
PRAI	CH 1978-2519		19780308		
	US 1979-14661		19790223		
	CS 1979-1460		19790305		
	AT 1979-1710		19790307		

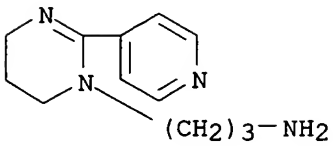
AB The antitumor (no data) compds. I (R = aryl, arylamino, aralkyl, arylaminoalkyl; R1 = aryl, arylamino; X = O, S; X1 = alkylene n = 1, 2) were prepd. Thus, 2,6-Cl2C6H3NHCH2CN was treated with HN(CH2CH2NH2)2 to give II (R2 = H), which was treated with 4-MeC6H4NCO to give II (R2 = CONHC6H4Me-4).

IT **73998-75-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(prepn. and reaction of, with isocyanates)

RN 73998-75-1 CAPLUS

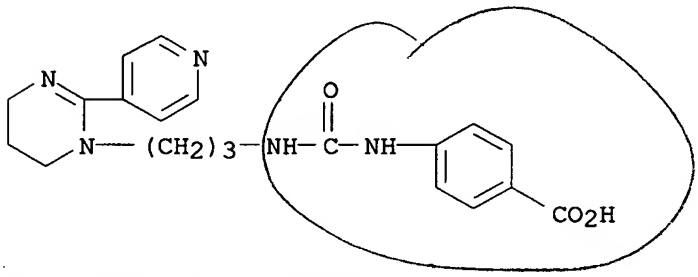
CN 1(4H)-Pyrimidinepropanamine, 5,6-dihydro-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)



IT **73998-73-9P 76692-14-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

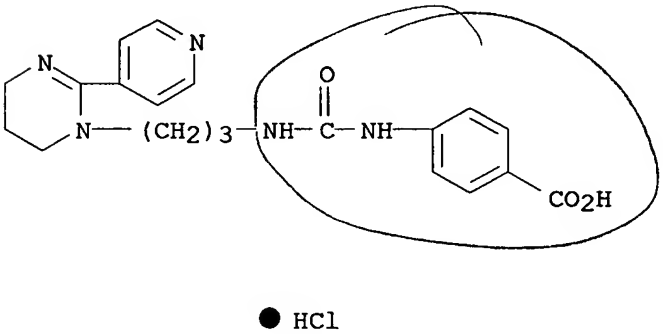
RN 73998-73-9 CAPLUS

CN Benzoic acid, 4-[[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 76692-14-3 CAPLUS

CN Benzoic acid, 4-[[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L17 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1980:446666 CAPLUS
DN 93:46666
TI Process for the preparation of novel imidazole urea and amido compounds
IN Marxer, Adrian
PA Ciba-Geigy A.-G., Switz.
SO Brit. UK Pat. Appl., 14 pp.
CODEN: BAXXDU
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2016011	A	19790919	GB 1979-8098	19790307
	GB 2016011	B2	19820825		
	CA 1125759	A1	19820615	CA 1979-321545	19790215
	US 4292429	A	19810929	US 1979-14661	19790223
	FI 7900740	A	19790909	FI 1979-740	19790305
	FI 70708	B	19860626		
	FI 70708	C	19861006		
	EP 4561	A2	19791017	EP 1979-100647	19790305
	EP 4561	B1	19811104		
	EP 4561	A3	19791114		
	R: BE, CH, DE, FR, GB, IT, LU, NL, SE				
	CS 244656	B2	19860814	CS 1979-1460	19790305
	ES 478342	A1	19790516	ES 1979-478342	19790306
	DD 142336	C	19800618	DD 1979-211405	19790306
	PL 116762	B1	19810630	PL 1979-213924	19790306
	PL 123150	B1	19820930	PL 1979-221681	19790306
	IL 56797	A1	19820930	IL 1979-56797	19790306
	DK 7900952	A	19790909	DK 1979-952	19790307
	NO 7900765	A	19790911	NO 1979-765	19790307
	NO 152606	B	19850715		
	NO 152606	C	19851023		
	AU 7944900	A1	19790913	AU 1979-44900	19790307
	AU 531006	B2	19830804		
	AT 7901710	A	19810315	AT 1979-1710	19790307
	AT 364375	B	19811012		
	SU 845779	A3	19810707	SU 1979-2733999	19790307
	HU 25271	O	19830628	HU 1979-CI1920	19790307
	HU 182940	B	19840328		
	JP 54125668	A2	19790929	JP 1979-26245	19790308
	JP 62009109	B4	19870226		
	SU 923367	A3	19820423	SU 1980-2872253	19800118
	AT 8003951	A	19810515	AT 1980-3951	19800730
	AT 365179	B	19811228		
	US 4420619	A	19831213	US 1981-247427	19810325
	CS 244700	B2	19860814	CS 1984-8407	19841105
PRAI	CH 1978-2519		19780308		
	US 1979-14661		19790223		
	CS 1979-1460		19790305		
	AT 1979-1710		19790307		

Same as #19

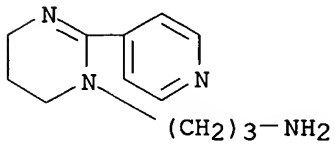
AB Ureas and amides I (R, R2 = monocyclic, carbocyclic aryl or heteroaryl; R1 = H, alkyl; n = 0, 1; m = 0, 1, 2; x = 1, 2; Z = alkylene having 2-3 C atoms in the linear chain; Z1 = O, S; Z2 = imino, bond) and I salts were prepd. E.g., 1-[2-[2-(2,6-dichloroanilinomethyl)-2-imidazolin-1-yl]ethyl]-3-(p-tolyl)urea was prepd. by stirring 1-aminoethyl-2-(2,6-dichloroanilinomethyl)-2-imidazoline with p-MeC6H4NCO in PhMe at

90.degree. for 3 h. I have a powerful action against tumors; their activities were assessed against respiratory carcinomas in golden hamsters and the Ehrlich ascites carcinoma in mice. They are particularly valuable for the treatment of bronchial carcinomas. Compns. contg. I are described.

IT **73998-75-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and addn. reaction of, with aryl isocyanate)

RN 73998-75-1 CAPLUS

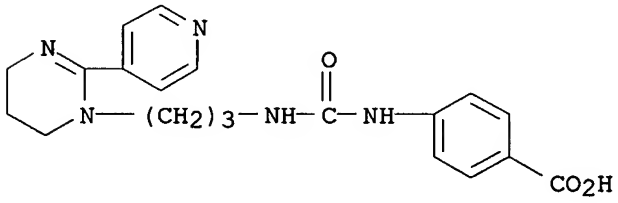
CN 1(4H)-Pyrimidinepropanamine, 5,6-dihydro-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)



IT **73998-73-9P 73998-74-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as neoplasm inhibitor)

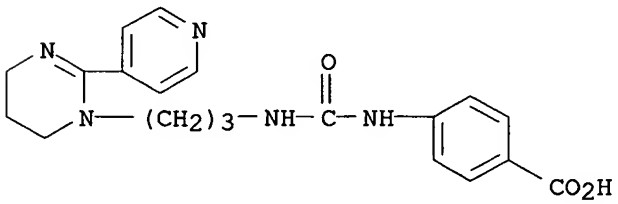
RN 73998-73-9 CAPLUS

CN Benzoic acid, 4-[[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 73998-74-0 CAPLUS

CN Benzoic acid, 4-[[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]-, hydrochloride (9CI) (CA INDEX NAME)



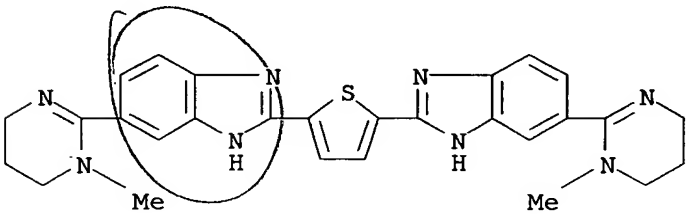
● x HCl

L17 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1979:38914 CAPLUS
DN 90:38914
TI Substituted bis(benzimidazolyl)thiophene compounds
IN Roesner, Manfred; Loewe, Heinz; Raether, Wolfgang
PA Hoechst A.-G., Fed. Rep. Ger.
SO Ger. Offen., 17 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2711362	A1	19780921	DE 1977-2711362	19770316
	ES 467739	A1	19790701	ES 1978-467739	19780310
	US 4156778	A	19790529	US 1978-886517	19780314
	CA 1095038	A1	19810203	CA 1978-298885	19780314
	NL 7802848	A	19780919	NL 1978-2848	19780315
	ZA 7801540	A	19790328	ZA 1978-1540	19780315
	AU 7834155	A1	19790920	AU 1978-34155	19780315
	GB 1599102	A	19810930	GB 1978-10291	19780315
	BE 864977	A1	19780918	BE 1978-186003	19780316
	FR 2383944	A1	19781013	FR 1978-7618	19780316
	JP 53135978	A2	19781128	JP 1978-30484	19780316
	ES 475989	A1	19790516	ES 1978-475989	19781214
PRAI	DE 1977-2711362		19770316		
	DE 1978-2804835		19780204		

AB Protozoacidal (no data) bis(benzinidazolyl)thiophenes I (RR1 = optionally substituted (CH2)2-4; R2 = H, alkyl, aminoalkyl, Ph) were prepd. Thus, 4,3-H2N(O2N)C6H3CN was subjected to alcoholysis with HOCH2CH2OMe and the resulting 4,3-H2N(O2N)C6H3C(:NH)OCH2CH2OMe treated with H2NCH2CHMeNH2 to give imidazoline II (R3 = NO2), which was reduced to II (R3 = NH2). Condensation of II (R3 = NH2) with the thiophenediimidate III gave I (RR1 = CHMeCH2, R2 = H). III was obtained by ethanolysis of 2,5-thiophenedicarbonitrile.

IT **68662-31-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 68662-31-7 CAPLUS
CN 1H-Benzimidazole, 2,2'-(2,5-thiophenediyl)bis[5-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)-, monohydrobromide (9CI) (CA INDEX NAME)

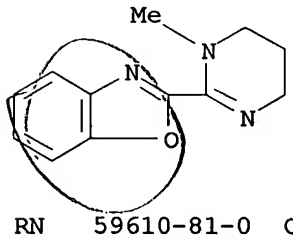


● HBr

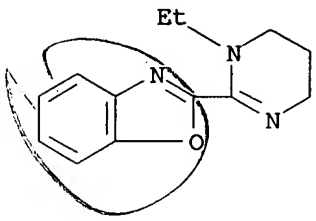
L17 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1976:432976 CAPLUS
DN 85:32976
TI Benzoxazol-2-yl-substituted imidazolines and tetrahydropyrimidines, and cosmetic compositions containing them
IN Moeller, Hinrich; Gloxhuber, Christian
PA Henkel und Cie. G.m.b.H., Fed. Rep. Ger.
SO Ger. Offen., 21 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE 2436279	A1	19760212	DE 1974-2436279	19740727
PRAI DE 1974-2436279		19740727		

AB Benzoxazoles I (X = CH2, R = H, Me, Cl, NO2, R1 = H; X = CH2, R = H, R1 = Me, CHMe2, Ph, CH2CH2OH; X = CHMe, CMe2, CH2CH2, CH2CH(OH), R = R1 = H; X = CH2CH2, R = H, R1 = Me, Et, cyclohexyl) were prepd. by condensing 2-cyanobenzoxazoles with R1NHXCH2NH2. I at 50-500 mg/kg orally gave 5.1-60.5% inhibition of dextran edema in rats. I are also uv absorbers, making them suitable for sunscreen prepns.
IT **59610-80-9P 59610-81-0P 59610-82-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antiinflammatory activity of)
RN 59610-80-9 CAPLUS
CN Benzoxazole, 2-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)



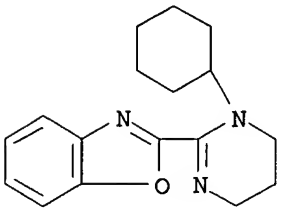
RN 59610-81-0 CAPLUS
CN Benzoxazole, 2-(1-ethyl-1,4,5,6-tetrahydro-2-pyrimidinyl)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 59610-82-1 CAPLUS

CN Benzoxazole, 2-(1-cyclohexyl-1,4,5,6-tetrahydro-2-pyrimidinyl)-, hydrochloride (9CI) (CA INDEX NAME)



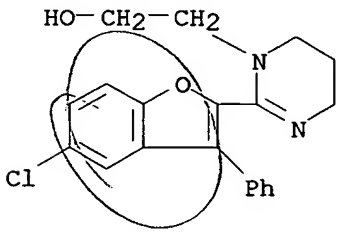
●x HCl

L17 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1976:90154 CAPLUS
DN 84:90154
TI Imidazolyl benzofurans
IN Brown, Richard E.; Shavel, John, Jr.
PA Warner-Lambert Co., USA
SO U.S., 8 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3927023	A	19751216	US 1974-473253	19740524
PRAI US 1974-473253		19740524		

AB Twenty-one imidazolyl- or pyrimidinylbenzofurans, most of them of structure I (R = H, Cl, Ph; R1 = H, Cl, OMe; R2 = H, Br, Cl; R3 = H, OH, Ph, p-ClC6H4, NH2; n = 0, 1), useful in the management of gastric hyperacidity and gastric ulcers (gastric antisecretory effect in rats given), were prepd. by reaction of phenols with BrCH2CN and treating the resulting phenoxyacetonitriles with H2NCH2CH2(CH2)nNH2 (n = 0,1). Thus, a mixt. of o-PhCOC6H4OH and BrCH2CN was stirred in Me2SO contg. K2CO3 for 5 hr at 75.degree. to give o-PhCOC6H4OCH2CN, which was heated with H2NCH2CH2NH2 in the presence of CS2 for 5 hr on a steam bath to give I (R = R1 = R2 = H; R3 = Ph; n = 0). Five other alkylenediamines (e.g., 2,3-diaminobutane, 2-hydroxy-1,3-propanediamine) were also used and gave the corresponding compds. with substituents on the N heterocycle moiety.

IT **58430-31-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 58430-31-2 CAPLUS
CN 1(4H)-Pyrimidineethanol, 2-(5-chloro-3-phenyl-2-benzofuranyl)-5,6-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L17 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1972:148743 CAPLUS
DN 76:148743
TI Anthelmintic activity in sheep of some compounds related to pyrantel and morantel
AU Austin, W. C.; Cornwell, R. L.; Jones, R. M.; Robinson, M.
CS Res. Div., Pfizer Ltd., Sandwich/Kent, UK
SO Journal of Medicinal Chemistry (1972), 15(3), 281-5
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English

Same as #25

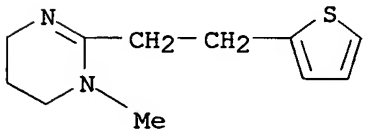
AB Pyrantel (I) [15686-83-6] (25 mg/kg) and morantel (II) [20574-50-9] (10 mg/kg) are the most active against major nematode infections in sheep (i.e. Haemonchus contortus, Trichostrongylus colubriformis, Nematodirus battus) compared with 34 cyclic amidines previously reported (McFarland, 1969, 1970) for the Nematospiroides dubius rodent screen. Structural characteristics of thienylvinyl cyclic amidines resulting in increased activity were; larger basic ring (n = 2), methylation of N (R1), maintenance of the trans vinyl linkage and 2-thienyl linkage. Replacement of the thiophene ring with a phenyl ring decreased activity; however, in a series of styryl tetrahydropyrimidines (III), ortho substitution with Me, Cl, and Br gave more active compds. in sheep than the unsubstituted compd. In a series of pyridinium salts (IV) most of the structure activity relations established in other series held true, but this series was less potent than the pyrantel series.

IT **5671-32-9 5722-14-5 26038-56-2**
32138-44-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anthelmintic activity of)

RN 5671-32-9 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (9CI) (CA INDEX NAME)

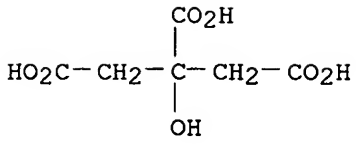
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

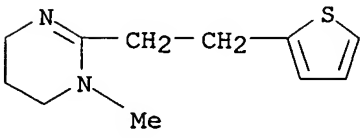
CRN 77-92-9
CMF C6 H8 O7



RN 5722-14-5 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

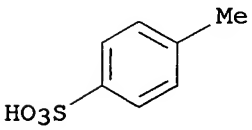
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

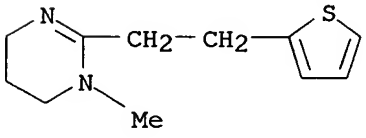
CRN 104-15-4
CMF C7 H8 O3 S



RN 26038-56-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

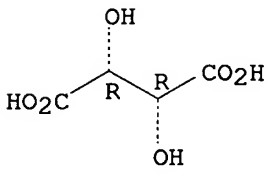
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 87-69-4
CMF C4 H6 O6

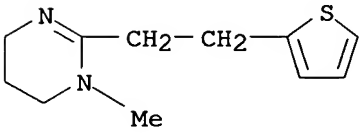
Absolute stereochemistry.



RN 32138-44-6 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

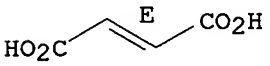
CRN 5685-90-5
CMF C11 H16 N2 S



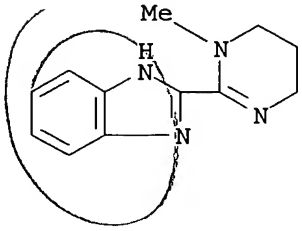
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



L17 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1972:99562 CAPLUS
DN 76:99562
TI Reactions of 2-benzimidazolecarbonitrile
AU Berndt, E. W.; Fratzke, H. A.; Held, B. G.
CS Res. Div., Salsbury Lab., Charles City, IA, USA
SO Journal of Heterocyclic Chemistry (1972), 9(1), 137-40
CODEN: JHTCAD; ISSN: 0022-152X
DT Journal
LA English
AB Cyclization occurred at the cyano group when 2-benz-imidazolecarbonitrile (I) was treated with diamines, aminoalcs. or aminothiols. Thus, I and EtNHCH2CH2NH2 gave 2-(1-ethyl-2-imidazolin-2-yl)benzimidazole. Similarly 6 analogs were prepd. I was converted to the thiocarboxamide, carboxamide and carboxamide oxime which in turn gave benzimidazoles substituted in the 2-positions by thiazole, oxazole, and 1,2,4-oxadiazole rings.
IT **35369-24-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35369-24-5 CAPLUS
CN 1H-Benzimidazole, 2-(1,4,5,6-tetrahydro-1-methyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1971:405937 CAPLUS
DN 75:5937
TI Anthelmintic 2-substituted-2-.DELTA.2-tetrahydropyrimidines and .DELTA.2-imidazolines
IN Conover, Lloyd H.; McFarland, James W.; Austin, William C.
PA Pfizer, Chas., and Co., Inc.
SO U.S., 14 pp.
CODEN: USXXAM
DT Patent
LA English

Same as #26

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3549624	A	19701222	US 1967-661220	19670817
PRAI US 1967-661220		19670817		

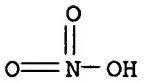
AB The title anthelmintic agents are prepd. Thus, a mixt. of 3-(2-thienyl)propionitrile, ethylenediamine (I), and p-MeC6H4SO3H.H2O is heated 8 hr at 175.degree. to give the toluenesulfonate salt which on treatment with alkali yields 2-[2-(2-thienyl)ethyl]-.DELTA.2-imidazoline, m. 99-101.degree.. Similarly, 2-[2-(2-thienyl)ethyl]-.DELTA.2-tetrahydropyrimidine is prepd. by substituting trimethylenediamine for I. An addnl. 29 examples are described plus formulations.

IT **5671-30-7P 5671-32-9P 5671-33-0P**
5685-90-5P 5722-14-5P 5822-06-0P
7660-04-0P 21913-62-2P 26038-56-2P
32079-85-9P 32079-86-0P 32079-87-1P
32079-88-2P 32080-96-9P 32080-97-0P
32138-43-5P 32138-44-6P 32434-91-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 5671-30-7 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, mononitrate (8CI, 9CI) (CA INDEX NAME)

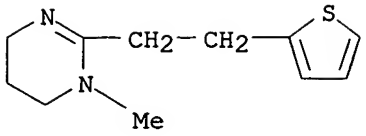
CM 1

CRN 7697-37-2
CMF H N O3



CM 2

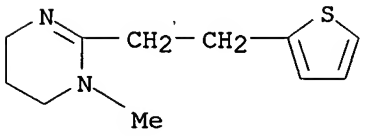
CRN 5685-90-5
CMF C11 H16 N2 S



RN 5671-32-9 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (9CI) (CA INDEX NAME)

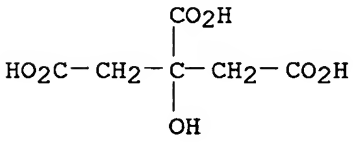
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S

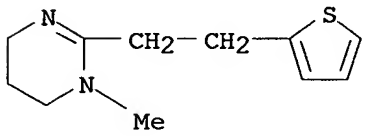


CM 2

CRN 77-92-9
CMF C6 H8 O7

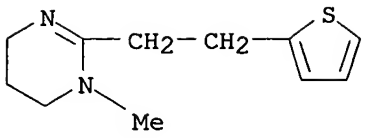


RN 5671-33-0 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)



● HCl

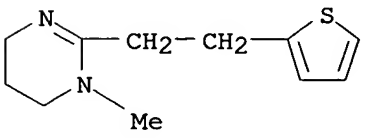
RN 5685-90-5 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]- (8CI, 9CI) (CA INDEX NAME)



RN 5722-14-5 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

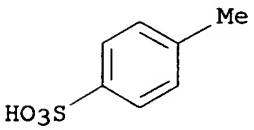
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

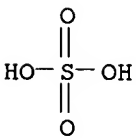
CRN 104-15-4
CMF C7 H8 O3 S



RN 5822-06-0 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, sulfate (1:1) (8CI, 9CI) (CA INDEX NAME)

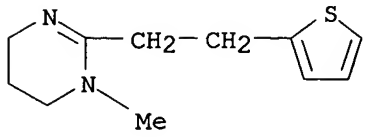
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

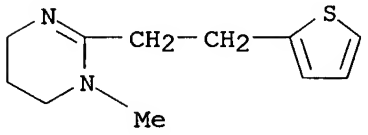
CRN 5685-90-5
CMF C11 H16 N2 S



RN 7660-04-0 CAPLUS
CN Benzoic acid, 2-hydroxy-5-sulfo-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

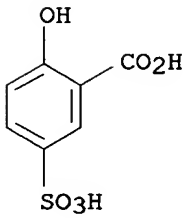
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

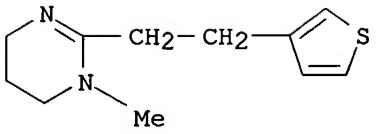
CRN 97-05-2
CMF C7 H6 O6 S



RN 21913-62-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(3-thienyl)ethyl]-, fumarate (1:1) (8CI) (CA INDEX NAME)

CM 1

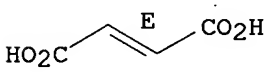
CRN 46328-63-6
CMF C11 H16 N2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

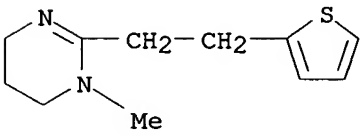
Double bond geometry as shown.



RN 26038-56-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

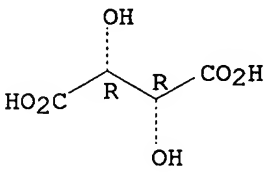
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 87-69-4
CMF C4 H6 O6

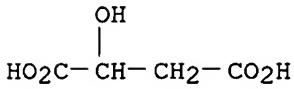
Absolute stereochemistry.



RN 32079-85-9 CAPLUS
CN Butanedioic acid, hydroxy-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

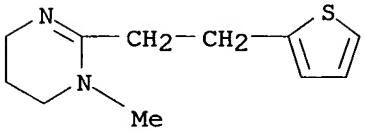
CM 1

CRN 6915-15-7
CMF C4 H6 O5



CM 2

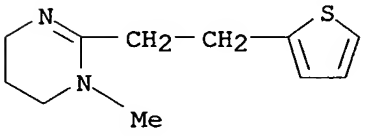
CRN 5685-90-5
CMF C11 H16 N2 S



RN 32079-86-0 CAPLUS
CN Butanedioic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

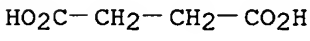
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 110-15-6
CMF C4 H6 O4

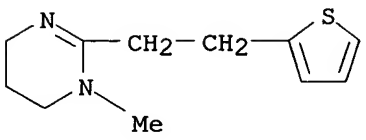


RN 32079-87-1 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, monoacetate (8CI, 9CI) (CA INDEX NAME)

CM 1

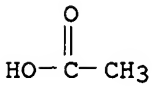
CRN 5685-90-5

CMF C11 H16 N2 S



CM 2

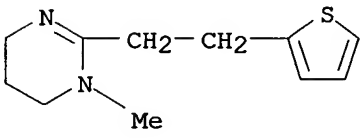
CRN 64-19-7
CMF C2 H4 O2



RN 32079-88-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

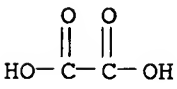
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

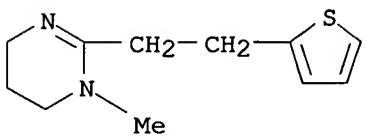
CRN 144-62-7
CMF C2 H2 O4



RN 32080-96-9 CAPLUS
CN 2-Naphthalenecarboxylic acid, 4,4'-methylenebis[3-hydroxy-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

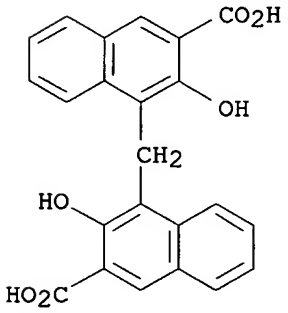
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

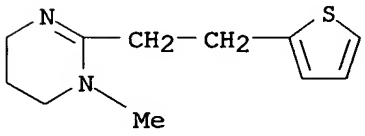
CRN 130-85-8
CMF C23 H16 O6



RN 32080-97-0 CAPLUS
CN Dodecanoic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

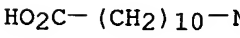
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

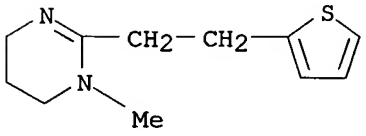
CRN 143-07-7
CMF C12 H24 O2



RN 32138-43-5 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

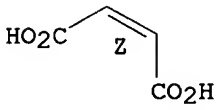
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

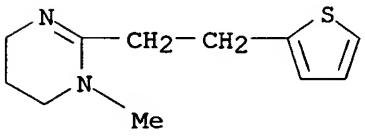
Double bond geometry as shown.



RN 32138-44-6 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

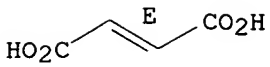
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

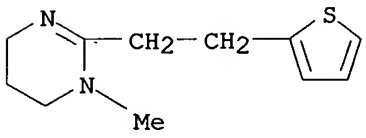
Double bond geometry as shown.



RN 32434-91-6 CAPLUS
CN Octadecanoic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

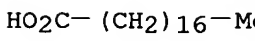
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 57-11-4
CMF C18 H36 O2



L17 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1970:475330 CAPLUS
DN 73:75330
TI Aspects of the pharmacology of a new anthelmintic: pyrantel
AU Aubry, M. L.; Cowell, Pauline; Davey, M. J.; Shevde, S.
CS Ther. Res. Div., Pfizer Group, Sandwich, UK
SO British Journal of Pharmacology (1970), 38(2), 332-44
CODEN: BJPCBM; ISSN: 0007-1188
DT Journal
LA English

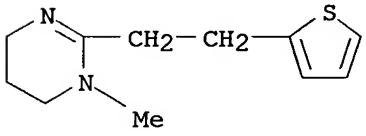
Same as #26

AB The pharmacol. properties of an anthelmintic, pyrantel, and some of its analogs have been described and compared with piperazine in a variety of vertebrate and helminth prepns. Pyrantel and its analogs in common with nicotine and decamethonium cause spastic paralysis in chicks and contracture of the chick semispinalis and toad rectus abdominis muscles. In the soleus and anterior tibialis muscles of the cat, pyrantel in large amts. caused a short-lived neuromuscular block that was preceded by initial depolarization. In prepns. from cat and rat, pyrantel showed properties common to both competitive and depolarizing neuromuscular blocking drugs. Pyrantel blocked the contracture evoked by transmural stimulation and caused a marked contracture of the worm. Piperazine caused a gradually developing redn. in the responses to transmural stimulation and no contracture. Pyrantel and its analogs caused a slowly developing contracture of strip prepns. of Ascaris, being more than 100 times more active than acetylcholine in this respect. Piperazine caused a relaxation of Ascaris strip prepns. and in common with (+)-tubocurarine blocked the responses to acetylcholine and pyrantel analogs on this prepn. Pyrantel caused depolarization and increased spike discharge frequency in single muscle cells of Ascaris, these changes being accompanied by increase in tension. Piperazine, on the other hand, caused hyperpolarization and redn. in spike discharge frequency and relaxation, and antagonized the effects of pyrantel.

IT **5671-37-4**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacology of)
RN 5671-37-4 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2R,3R)-2,3-dihydroxybutanedioate (9CI) (CA INDEX NAME)

CM 1

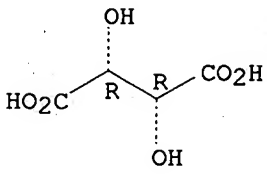
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.



L17 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1969:430487 CAPLUS
DN 71:30487
TI Anthelmintic thiophene derivatives
IN Austin, William C.; Conover, Lloyd H.; McFarland, James W.
PA Pfizer Ltd.
SO Brit., 5 pp. Addn. to Brit. 1045838
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1145867		19690319	GB	19661019
	FR 7532			FR	

AB Addn. to Brit. 1,045,838 (See Belg. 658,987, CA 64: 8192c). The title compds. (I) are prepd. Thus, a mixt. of 9.77 g. 3-formylthiophene (II), 9.59 g. 1,2-dimethyl-1,4,5,6-tetrahydropyrimidine (III), and 75 ml. dry PhMe is refluxed 6 hrs. in an app. with moisture trap, the mixt. decanted from a small amt. black tar, the PhMe distd. in vacuo, and the residual crude base poured into a soln. of 11.14 g. fumaric acid (IV) in 40 ml 1:1 aq. iso-Pr gives the fumarate of trans-1-methyl-2-[2-(3-thienyl)vinyl]-1,4,5,6-tetrahydropyrimidine, m. 192.5-94.degree. (iso-PrOH), which may be converted to the cis form by irradn. A Grignard reagent, prepd. by refluxing 72 hrs. a mixt. of 76 g. 2,3-dibromothiophene, 22 g. EtBr, 13.2 g. Mg, 800 ml. dry Et2O, and a few crystals iodine, is poured into a stirred mixt. (cooled in ice) of 52 g. HCONMe2 and 200 ml. Et2O, the mixt. refluxed 2 hrs., dil. HCl added (stirring), and the mixt. worked up to give 42 g. 3-bromo-2-formylthiophene (V), b19 121-3.degree., n21D 1.6355. A mixt. of 7.4 g. III, 12 g. V, and 60 ml. PhMe is refluxed 4 hrs. in an app. with moisture trap, the PhMe distd. in vacuo, the residual crude base treated with a soln. of 15 g. tartaric acid in 50 ml. 1:1 aq. iso-PrOH, and the mixt. kept 16 hrs. at 0.degree. to give 1-methyl-2-[2-(3-bromo-2-thienyl)vinyl]-1,4,5,6-tetra-hydropyrimidine tartrate monohydrate, m. 110.5-13.degree. (H2O-iso-PrOH, then MeOH-Et2O). A mixt. of 42 g. dry EtCH(CO2Na)CH2CO2Na, 45 g. P4S7, and 75 ml. high b.p. mineral oil is added over 2 hrs. to 50 ml. mineral oil at 250-300.degree. under CO2 and the distillate fractionated to give 3-ethylthiophene (VI), b. 143-5.degree.. POCl3 20 g.) is added over 0.5 hr. to a stirred, heated (steam-bath) mixt. of 11.2 g. VI and 8.4 g. HCONMe2, heating continued 1 hr., the mixt. cooled and poured into 150 ml. ice-H2O, NaOAc added to pH 5, and the mixt. worked up to give a 5:2 mixt. (VII) of 3- and 4-ethyl-2-formylthiophene, b17 114-6.degree.. A mixt. of 9.8 g. VII, 7.9 g. III, and PhMe contg. a few drops piperidine is refluxed 6 hrs., the PhMe distd. in vacuo, the residual crude base dissolved in a hot soln. of 8.5 g. IV in 15 ml. H2O, 40 ml. iso-PrOH added, and the soln. cooled to give 4.5 g. trans-1-methyl-2-[2-(3-ethyl-2-thienyl)vinyl]-1,4,5,6-tetra-hydropyrimidine, m. 166-71.degree. (H2O-iso-PrOH). A mixt. of 24.89 g. II, 21.20 g. cyanoacetic acid 0.80 g. NH4OAc, 27.5 ml pyridine, and 80 ml. dry xylene is refluxed 17 hrs. to give a cis-trans mixt. of 3-(3-thienyl)acrylonitrile (VIII), b1.cntdot.5 102-8.degree.. A mixt. of 16 g. VIII, 300 ml. MeOH, and 2.9 g. 10% Pd-C is hydrogenated 6 hrs. under superatm. pressure and room temp. and worked up to give 3-(3-thienyl)propionitrile (IX), b14, 136-8.degree.. Et 3-(3-thienyl)propionimidate-HCl [m. 114-5.degree. (decompn.), prepd. from IX, EtOH, and HCl] (3.5 g.) is added to a soln. of 1.4 g. MeNH(CH2)3NH2 in 25 ml. EtOH at room temp., the mixt. refluxed 3 hrs. and evapd. to dryness in vacuo, the residue extd. with CH2Cl2 after making alk. with ice-cold

aq. NaOH soln. and worked up, and the residue (2.4 g.) dissolved in 15 ml. MeOH and the soln. treated with 1.45 g. IV to give 1-methyl-2-[2-(3-thienyl)ethyl]-1,4,5,6-tetrahydropyrimidine fumarate, m. 165-6.degree. (MeOH). I are effective against Trichostrongylus species of helminth order Strongylidae found in stomachs and intestines of sheep and cattle, and are administered at a daily rate of 1-150 mg./kg. (therapy, 1-4 days) or 1-50 mg./kg. (prophylaxis). Examples (4) of veterinary compns. are given.

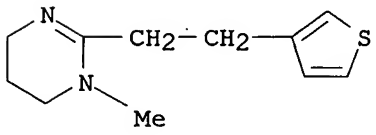
IT **22827-72-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 22827-72-1 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(3-thienyl)ethyl]-, fumarate (8CI) (CA INDEX NAME)

CM 1

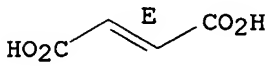
CRN 46328-63-6
CMF C11 H16 N2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



L17 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1969:413126 CAPLUS
DN 71:13126
TI 2-(1-Isochromanyl)-heterocycles
IN Faust, John A.; Sahyon, Melville
PA Sahyun Laboratories
SO U.S., 7 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

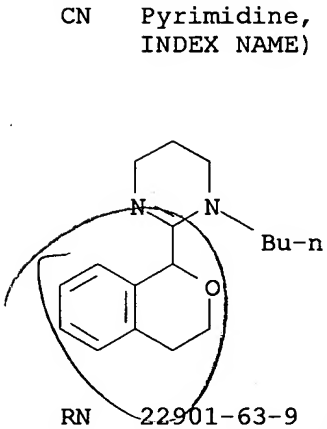
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3438995	A	19690415	US 1968-696145	19680108
PRAI US 1968-696145		19680108		

AB HCl was bubbled through 244 g. PhCH2CH2OH2OH and 75 g. paraformaldehyde at 0-10.degree. until the mixt. was homogeneous, 20% NaOH added, and the mixt. refluxed 1 hr. and worked up to give 250 g. isochroman (I), b19 100-3.degree.. To I in CCl4 at 10.degree. under uv light was added over 3 hrs. 1 equiv. Br in CCl4 to give crude 1-bromoisochroman, which refluxed 16 hrs. with CuCN in PhMe gave 63% 1-cyanoisochroman (II), b0.4 93-5.degree.. II with 1 equiv. H2N(CH2)2NH2 mono-p-toluenesulfonate (TsOH) at 140-50.degree. under N 2 hrs. gave 43% 2-(1-isochromanyl)-2-imidazoline (III), m. 121-3.degree.; HCl salt m. 230-2.degree. (decompn.). Similarly, 6.4 g. II with 1 equiv. H2N(CH2)3NH2.TsOH gave 6 g. 2-(1-isochromanyl)-1,4,5,6-tetrahydropyrimidine (IV); HCl salt m. 236-7.degree. (decompn.); 10.8 g. 1-butyl-1-cyanoisochroman (V) and 1 equiv. TsOH gave 4.6 g. 2-[1-(1-butyl)isochromanyl]-2-imidazoline, b0.3 150-2.degree. (H2SO4 salt, m. 175-7.degree.); 6 g. II with 1 equiv. BuNH(CH2)3NH2.TsOH gave 4.4 g. 1-butyl deriv. of IV, b0.8 165-7.degree.; 7 g. II with 1 equiv. (H2NCH2)2CHOH.TsOH gave 13 g. 5-hydroxy deriv. of IV, m. 192-3.degree. (HCl salt, m. 263-4.degree.); 6 g. II with 1 equiv. HO(CH2)2NH(CH2)2NH2.TsOH gave 5 g. 1-(2-hydroxyethyl) deriv. of IV, m. 156-8.degree.. II (16 g.) and 13.7 g. BuBr in C6H6 added dropwise to 4.3 g. 90% NaNH2 in C6H6 and the mixt. refluxed 1.5 hrs. gave 13.3 g. V, b0.7 118-20.degree.. Similarly, 8 g. II with 9 g. tetrahydropyran-2-yl 3-chloropropyl ether gave 8.3 g. tetrahydropyran-2-yl 3-(1-cyanoisochroman-1-yl)propyl ether (VI), b0.5 188-90.degree.. IV (5 g.) with 2.5 ml. 37% HCHO in EtOH kept 24 hrs. at 25.degree. gave 2.5 g. 1-hydroxymethyl deriv. of III, m. 221-2.degree.. II (6 g.) and 3.3 g. 1,3-diaminobutane was treated with 300 mg. H2S, and heated 2 hrs. at 145.degree. to give 2.5 g. 4-Me deriv. of IV, b0.2 147-53.degree.; HCl salt, m. 243-5.degree. (decompn.). Similarly, 6 g. II with 1 equiv. (H2NC2H4)2 gave 2.5 g. 1-(2-aminoethyl) deriv. of III; 2HCl salt m. 283-5.degree. (decompn.); 6 g. II with 3 g. MeNHC2H4NH2 (VII) gave 1.7 g. 1-Me deriv. of IV, b0.3 134-7.degree., m. 95-7.degree.; 10.5 g. VI with 1 equiv. VII gave 2.4 g. 2-[1-(1-butyl)isochromanyl]-1-methyl-2-imidazoline, b0.2 142-4.degree.; 4.9 g. VI with 1 g. H2NC2H4NH2 gave 0.7 g. 2-[1-(3-hydroxypropyl)-1-isochromanyl]-2-imidazoline, m. 140-1.degree.. The diazonium salt from 19.5 g. 4-aminohomophthalic acid and 7 g. NaNO2 in HCl was added to 12.4 g. Cu2Cl2 in 25 ml. 36% HCl and 10 ml. H2O at 0.degree. to give 16.4 g. 4-chlorohomophthalic acid, m. 196-7.degree.. This (60 g.) in 50 ml. EtOH and 90 ml. C6H6 with 0.5 ml. 98% H2SO4 refluxed overnight (H2O separator) gave 23.3 g. di-Et 4-chlorohomophthalate, b0.8 140-2.degree.. This (23.2 g.) with 3.8 g. LiAlH4 in Et2O gave 11.5 g. 4-chloro-2-hydroxymethylphenethyl alc., m. 75-6.degree., which heated with 85% H3PO4 at 95-100.degree. 4 hrs. gave 98% 7-chloroisochroman, b24 139-40.degree.. This (4.9 g.) in CCl4 under uv light treated dropwise with 4.8 g. Br in

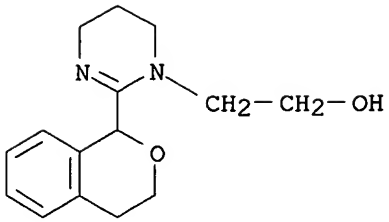
CCl4 gave 7.8 g. 1-bromo-7-chloroisochroman, m. 110-15.degree., which with 4.0 g. CuCN in PhMe gave 3.8 g. 7-chloro-1-cyanoisochroman, m. 112-14.degree.. This (3.8 g.) heated with 5.8 g. TsOH 2 hrs. at 200.degree. gave 0.3 g. 2-(7-chloro-1-isochromanyl)-2-imidazoline, m. 119-21.degree.. Addn. of 160 g. Br in CCl4 dropwise to 134 g. I in CCl4 cooled in ice and under uv light, then distn. gave 180 g. o-(.beta.-bromoethyl)benzaldehyde, b0.3 90-2.degree.. This (18.6 g.) and 14.7 g. BrCH2CO2Et in dry Et2O added to 10 g. Zn dust in Et2O and the mixt. refluxed 4 hrs. gave 22 g. Et 3-hydroxy-3-0-(.beta.-bromoethyl)phenylpropionate, m. 64-5.degree., which with KOH in MeOH gave 1-isochromanylacetic acid, b0.4 155-7.degree., m. 69-71.degree.. This (7.5 g.) treated with 30 ml. SOCl2 and then NH4OH gave 7.3 g. 1-isochromanylacetamide, m. 109-10.degree., which was refluxed with SOCl2 in CHCl3 14 hrs. to give 1-isochromanylcarbonitrile, b0.3 124-6.degree.. This and H2NC2H4NH2 treated with H2S and the mixt. heated 45 min. at 115.degree. gave 2-(isochroman-1-ylmethyl)-2-imidazoline, b0.35 160.degree.; H2SO4 salt, m. 157-8.degree.. I (75 g.) with 600 ml. 48% HBr and 400 ml. HOAc refluxed 6 hrs. gave 66 g. o-(2-bromoethyl)benzyl bromide, b1.3 124-6.degree., which in Me2CO was added dropwise over 45 min. to Na2S.9H2O in iso-PrOH-H2O and the mixt. refluxed 4 hrs., then steam distd. to give isothiochroman, b19 130-5.degree.. This (11 g.) in CCl4 at -20.degree. treated over 30 min. with 5.3 g. Cl in CCl4 gave the crude 1-chloro deriv., which was added to 12 g. Hg(CN)2 and 10 g. CuCN in C6H6 and the mixt. refluxed 2 hrs. to give 4.2 g. 1-cyano analog, m. 66-7.degree.. This (4.2 g.) and 1.8 g. H2NC2H4NH2 treated with H2S, the mixt. heated 2 hrs. at 90-100.degree., and the crude product treated with HCl in EtOH gave 3 g. 2-(1-isothiochromanyl)-2-imidazoline-HCl, m. 226-8.degree. (decompn.). Title compds. possess anti-inflammatory and central nervous system depressant activities.

IT **22901-59-3P 22901-63-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 22901-59-3 CAPLUS
CN Pyrimidine, 1-butyl-1,4,5,6-tetrahydro-2-(1-isochromanyl)- (8CI) (CA INDEX NAME)



RN 22901-63-9 CAPLUS
CN 1(4H)-Pyrimidineethanol, 5,6-dihydro-2-(1-isochromanyl)- (8CI) (CA INDEX NAME)



L17 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1969:96809 CAPLUS
DN 70:96809
TI Pyrimidinyl vinyl thiophenes anthelmintics
IN Conover, Lloyd H.; McFarland, James W.; Austin, William C.
PA Pfizer Corp.
SO S. African, 15 pp.
CODEN: SFXXAB
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI ZA 6706178		19680807		
PRAI GB		19661019		

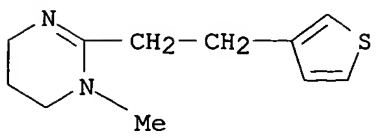
Same as #26

AB The prepn. of certain I and their addn. salts, effective as antihelmintic agents in sheep and cattle, is described. Thus, a mixt. of 0.1 mole 2-methyl-3-thiophenecar-boxaldehyde, 0.1 mole 1,2-dimethyl-.DELTA.2-tetrahydropyrimidine (II), and 100 ml. PhMe was refluxed 6 hrs., stripped of solvent, and poured into 40 ml. 1:1 water-iso-PrOH contg. 0.11 mole fumaric acid to give I. fumarate (R = R1 = Me, n = 2, Y = CH:CH). Similarly prepd. were the fumarate salts of I (R = Me, R1 = Cl, n = 1, Y = CH:CH), I(R = Me, R1 = Br, n = 2, Y = CH:-CH), and I (R = H, R1 = Et, n = 1, Y = CH:CH). A mixt. of 42 g. di-Na ethylsuccinate, 45 g. P4S7, and 75 ml. mineral oil was added over 2 hrs. to 50 ml. mineral oil at 250-300.degree. under CO2 to give 3-ethylthiophene (III), b. 143-5.degree.. POCl3 (20 g.) was added in 30 min. to 11.2 g. III and 8.4 g. HCONMe2 on a steam bath and the mixt. was heated 1 hr., poured into 150 ml. ice water, and adjusted to pH 5 with NaOAc to give a mixt. (IV), b17 114-16.degree., of 3-ethyl-2-thiophenecarboxaldehyde and the 5-ethyl isomer in the proportion 5:2. IV (9.8 g.) was refluxed 6 hrs. with 7.9 g. II as above to give V fumarate (R = Me, R1 = Et, n = 2, Y = CH:CH), m. 166-71.degree.. Also prepd. similarly were the fumarates of V (R = H, R1 = Et, n = 1, Y = CH:CH), V (R = H, R1 = Et, n = 2, Y = CH:CH), and V (R = Me, R1 = Et, n = 1, Y = CH:CH). A mixt. of 24.9 g. 3-thiophenecar-boxaldehyde, 21.2 g. NCCH2CO2H, 0.8 g. NH4OAc, 27.5 ml. pyridine, and 80 ml. xylene was refluxed 17 hrs. to give 3-(3-thienyl)-acrylonitrile (VI), b1.5 102-8.degree.. A mixt. of 16 g. VI, 300 ml. MeOH, and 2.9 g. 10% Pd-C was hydrogenated 6 hrs. at room temp. to give 3-(3-thienyl)propionitrile, b14 136-8.degree., from which ethyl 3-(3-thienyl)propionimidate-HCl (VII) was prepd. VII (3.5 g.) was added to 1.4 g. N-methyltrimethylenediamine in 25 ml. EtOH and the mixt. was refluxed 3 hrs. and treated with fumaric acid to give I fumarate (R = Me, R1 = H, n = 2, Y = CH2CH2), m. 165-6.degree.. Similarly prepd. were the fumarates of I (R = H, R1 = F, n = 1, Y = CH2CH2), I [R = R1 = Me, n = 1, Y = (CH2)3], l [R = Me, R1 = Cl, n = 1, Y = (CH2)3], V (R = H, R1 = Br, n = 2, Y = CH2CH2), V (R = H, R1 = Et, n = 1, Y = CH2CH2), and V [R = Me, R1 = Cl, n = 2, Y = CH2CH2). These compds. may be administered to animals as tablets or mixts. with mineral supplements or nutrient materials.

IT **21913-62-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 21913-62-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(3-thienyl)ethyl]-, fumarate (1:1) (8CI) (CA INDEX NAME)

CM 1

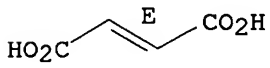
CRN 46328-63-6
CMF C11 H16 N2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



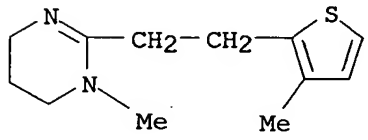
L17 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1969:47483 CAPLUS
DN 70:47483
TI 2-[.omega.-(3-Methyl-2-thienyl)alkyl]- and 2-[2-(3-methyl-2-thienyl)vinyl]-.DELTA.2-tetrahydropyrimidines and -.DELTA.2-imidazolines
IN Austin, William C.; Conover, Lloyd H.; McFarland, James W.
PA Pfizer Corp.
SO S. African, 32 pp.
CODEN: SFXXAB
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI ZA 6602855		19680104	ZA	19660517
DE 1745778			DE	

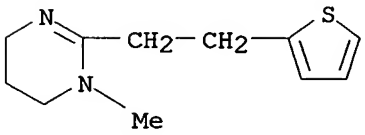
same as #26

AB The title compds. (I) are prepd. by (a) reaction of an alkylenediamine tosylate with the desired .omega.-(3-methyl-2-thienyl)-substituted nitrile (II) or (b) the imino-ether-HCl of II is reacted with an alkylenediamine (III) or (c) an ester of .omega.-(3-methyl-2-thienyl)alkanoic acid is reacted with III. When X is vinylene, I is also prepd. by reaction of (3-methyl-2-thienyl)-acrylamide with 1,3-propanesultone to give 3-[1-imino-3-(3-methyl-2-thienyl)alkyloxy]propanesulfonic acid which is then reacted with III. Thus, a soln. of 1.1 moles of 3-methylthiophene-2-carboxaldehyde, 1.0 mole NCCH2CO2H, 3 g. NH4OAc, 110 ml. pyridine, and 200 ml. toluene was heated 48 hrs. to give a colorless oil, 3-(3-methyl-2-thienyl)acrylonitrile (IV), b0.05-0.10 76.degree., n2D4 1.6330. IV was hydrogenated to give 3-(3-methyl-2-thienyl)propionitrile, b0 08-0.10 66.degree.. To 31.8 g. Me .beta.-(3-methyl-2-thienyl)propionimidate-HCl is added a soln. of 18.5 g. MeNH(CH2)3NH2 in 250 ml. MeOH at 0.degree. and refluxed. The free base reacted with an equimolar amt. of hexafluorophosphoric acid to give I (X = CH2CH2, R = Me, n = 2) hexafluoro-phosphonate salt, m 116.5-17.5.degree.. Similar I prepd. were (X, R, n, m.p., and salt given): CH:CH, H, 2, 239-41.degree., HCl: CH2CH2, Me, 1, - (oil), -

IT **21786-23-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 21786-23-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(3-methyl-2-thienyl)ethyl]-(8CI) (CA INDEX NAME)



L17 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1967:54143 CAPLUS
DN 66:54143
TI Pyrantel tartrate, a new anthelmintic effective against infections of domestic animals
AU Austin, William C.; et al.
CS Chem. Res. Dep., Pfizer, Ltd., Sandwich, UK
SO Nature (London, United Kingdom) (1966), 212(5067), 1273-4
CODEN: NATUAS; ISSN: 0028-0836
DT Journal
LA English
AB Six compds. of the general structure I were prepd., where R = H, R1 = H, X = CH2CH2, n = 2; R = H, R1 = H, X = CH2CH2, n = 3; R = H, R1 = Me, X = CH2CH2, n = 2; R = H, R1 = Me, X = CH2CH2, n = 3; R = H, R1 = Me, X = CH:CH, n = 3; and R = Me, R1 = Me, X = CH:CH, n = 3. All compds. had broad spectrum activity against both adult and immature worm infections of domestic animals. The activity of these compds. against Nematospiroides dubius in mice and Nippostrongylus muris in rats increased in the order in which the compds. are listed. 1,4,5,6-Tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine, administered in a single oral dose of 25 mg./kg., had a high level of activity against adult and immature Haemonchus, Ostertagia, and Trichostrongylus in the abomasum, and Nematodirus, Cooperia, and Trichostrongylus in the small intestine of both sheep and cattle, and had a therapeutic index of 7 in sheep. This compd. also was active against A scaris suum in pigs, and against Toxocara and Toxascaris in dogs, and virtually eliminated Anclyostoma caninum and Uncinaria stenocephala from dogs.
IT **5685-90-5**
RL: BIOL (Biological study)
(as anthelmintic)
RN 5685-90-5 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]- (8CI, 9CI) (CA INDEX NAME)



L17 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1966:43855 CAPLUS
DN 64:43855
OREF 64:8192c-h,8193a-c
TI Anthelmintic 2-alkylthiophenes
PA Pfizer Corp.
SO 47 pp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	BE 658987		19650728	BE	
	GB 1045838			GB	
PRAI	GB		19640128		

AB A mixt. of 123.5 g. 2-thiophenecarboxaldehyde, 85.0 g. NCCH2CO2H, 110 ml. C5H5N, 3 g. NH4OAc, and 200 ml. PhMe was refluxed under a Dean and Stark head for 48 hrs., the mixt. becoming very dark. Distn. gave 107.4 g. 3-(2-thienyl)acrylonitrile (I), b30 154.degree., n25D 1.6373. Catalytic hydrogenation 67.6 g. I in 300 ml. MeOH contg. 50 ml. N NaOH using 10 g. 10% Pd-C gave 49.5 g. 3-(2-thienyl)propionitrile (II), b35 156-8.degree., n25D 1.5372. Heating a mixt. of 13.7 g. II, 6.5 g. H2N(CH2)2NH2 (III), and 19.0 g. p-MeC6H4SO3H.H2O at 175.degree. for 8 hrs. and cooling gave 19.5 g. IV (n = 2, m = 1) (V) p-toluenesulfonate, m.104-6.degree. (iso-PrOH), converted into the free base, m. 99-101.degree. (Me2CO-C6H14). A mixt. of 8.5 g. Me, .beta.-(2-thienyl)propionimidate-HCl (VI), 2.7 g. III, and 40 ml. dry MeOH was refluxed for 90 min. to give V HCl salt, m. 142.5-3.5.degree. (iso-PrOH-Et2O). Similarly were prepd. IV (n = 2, m = 3) (VIa).HCl, m. 166.5-7.5.degree. from VI and H2N(CH2)3NH2, and IV (n = 3, m = 3) (VII), m. 138-9.degree. from Me.gamma.-(2-thienyl)butyrimidate-HCl. V pamoate and VII citrate were prepd. by mixing the components in EtOH and H2O, resp., and evapg. the solns. so formed. A mixt. of 23.4 g. 2-thienylacrylamide and 18.7 g. 1,3-propane sultone was heated with vigorous stirring at 130-40.degree. for 30 min. when the melt had solidified. Heating for a further 30 min., trituration with Me2CO, and filtering gave 38.9 g. 3-[1-imino(3-thienyalyloxy)propane]sulfonic acid, 3.2 g. of which when heated with 1.5 g. MeNH(CH2)3NH2 (VIIa) in 50 ml. EtOH for 90 min. under reflux, and treating with NaOH gave 1.3 g. VIII (R = Me, m = 2), m. 178-9.degree. (MeOH). The following VIII were similarly prepd. (R, m, salt, and m.p. given): H, 2, maleate, 153-5.degree.; Me, 1, p-toluenesulfonate, 162-4.degree.; H, 1, maleate, 162-3.degree.. The following IX were prepd. using the methods described (R, n, m, salt, and m.p. or b.p. given): Me, 2, 1, base (X), 134-6.degree./0.5 mm., (n24D 1.5570); Me, 2, 2, base (XI), 122-3.degree./0.4 mm., (n24D 1.5648); Me, 2, 1, p-toluenesulfonate, 104-5.5.degree. (iso-PrOH-Et2O); Me, 2, 1, citrate, 141-2.degree. (MeOH-Et2O); Me, 2, 1, phosphate, 191-2.5.degree.; Me, 2, 1, sulfate, 74.5-5.degree. (iso-PrOH); Me, 2, 2, p-toluenesulfonate (XII), 122-3.degree. (iso-PrOH-Et2O); Me, 2, 2, sulfate, 97-9.degree. (iso-PrOH); Me, 2, 2, nitrate, 108.5-110.degree. (iso-PrOH-Et2O); Me, 2, 2, 5-sulfosalicylate, 154-5.degree. (iso-PrOH); Me, 2, 2, citrate, 142-3.5.degree.; Me, 2, 2, phosphate, 202.5-5.degree. Me, 2, 2, HCl, 113-18.degree. (hygroscopic). Other salts of IX (R = Me, n = m = 2) prepd. were (salt and m.p. given): pamoate, 137-43.degree.; maleate, 78-80.degree.; stearate, 48-53.degree.; laurate, oil; tartrate, 140-2.degree.; malate, 99-100.degree.; fumarate, 149-51.degree.; succinate, 85-90.degree.; acetate, oil; oxalate, 76-8.degree.. Other salts of IX (R = Me, n = 2, m = 1) (salt and m.p. given): HCl, 70-90.degree.; sulfosalicylate, 153-9.degree.; pamoate, 166-8.degree.;

stearate, 48-53.degree.; laurate, oil; tartrate, 167-91.degree.; fumarate, 157-8.degree.; succinate, 107-8.degree.; acetate, oil. To a Grignard soln. prepd. by refluxing together for 2 hrs. 4.8 g. Mg, 28.7 g. 2-(2-chloroethyl)thiophene, and 200 ml. Et2O was slowly added a soln. of 23 g. Cl(CH2)4CN in 150 ml. dry Et2O. After refluxing 30 min., 150 ml. xylene was added, the ether removed, and the mixt. refluxed for 1 hr., cooled, and treated with 150 ml. 10% NH4Cl to give XIII (R = H, n = 2), b0.002 68-9.degree.; p-toluenesulfonate m. 101-3.degree. (iso-PrOH-Et2O); maleate m. 78-80.degree.. By a similar procedure were prepd. XIII (R = H, n = 1), b0.4 89.degree. (p-toluenesulfonate m. 100-1.5.degree.), and XIII (R = Me, n = 1), b0.5 97.9.degree. (p-toluenesulfonate m. 105-6.5.degree.. The amsonate of XI, m. >300.degree., was prepd. by treatment of a soln. of 1.85 g. amsonic acid in H2O contg. 2 equivs. NaOH with 3.8 g. XII in H2O. The suramin salt of VIa, m. 145-50.degree., was obtained as an amorphous solid from the components. VIa amsonate m. >300.degree.. A mixt. of 250 g. II and 160.5 g. VIIa was treated with H2S until 6.1 g. had been absorbed and the temp. was raised to 70-80.degree. for 2 hrs. and to 95.degree. for 6 hrs. Distn. gave 84.7% X. A similar yield was obtained using P2S5 in place of the H2S. 2-(2-Chloroethoxy)tetrahydropyran (XIV), b14 87-90.degree. was prepd. in 85.2% yield by reacting 241.5 g. Cl(CH2)2OH, 252 g. dihydropyran, and 10 drops concd. HCl. To 1.5 l. anhyd. liquid NH3 contg. 0.6 g. Zn(NO3)2 was added 32.9 g. Na followed dropwise by 78.7 g. EtCN followed by 266 g. XIV. Evapn., extn. with C6H6, and distn. gave 22.8% 2-(3-cyanobutoxy)tetrahydrofuran (XV), b15 95-102.degree.. Refluxing 59.8 g. XV in 150 ml. MeOH with 15 ml. concd. HCl for 5 min. gave 25 g. NCCHMeCH2CH2OH, b16 116-18.degree., which with 33 g. SOCl2 in 100 ml. C6H6 in the cold gave 15.6 g. NCCHMeCH2CH2Cl, b15 80-1.degree.. The compds. are active against helminths of the families Ancylostomatidae, Strongylidae, and Trichostrongylidae in sheep, cattle, goats, dogs, cats, and horses by the oral or parenteral routes and details are given. Laboratory expts. using mice and rats infected with Nematospiroides dubius, Nippostrongylus muris, and Syphacia obvelata are given in detail demonstrating therapeutic activity. Animals usually require only one dose, preferably parenterally, at a level of 20-150 mg. of the active base/kg. Oral doses are in the range 5-150 mg./kg. These compds. may also be used prophyllactically at a dosage of 5-50 mg./kg.

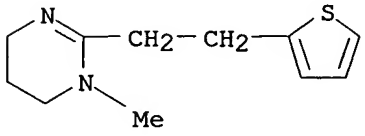
IT **5671-32-9**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, citrate (1:1) **5671-34-1**, 2-Naphthoic acid, 4,4'-methylenebis[3-hydroxy-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine **5671-35-2**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, maleate **5671-36-3**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, stearate **5671-37-4**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, tartrate **5671-38-5**, Malic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine **5671-39-6**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, fumarate **5671-40-9**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, succinate **5671-41-0**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, acetate **5685-90-5**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]- **5707-82-4**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, oxalate **5722-14-5**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, p-toluenesulfonate **7660-04-0**, Salicylic acid, 5-sulfo-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1)
(prepn. of)

RN 5671-32-9 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (9CI) (CA INDEX NAME)

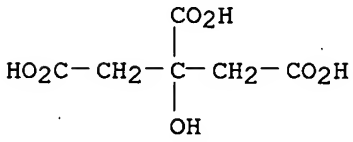
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

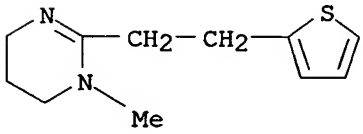
CRN 77-92-9
CMF C6 H8 O7



RN 5671-34-1 CAPLUS
CN 2-Naphthoic acid, 4,4'-methylenebis[3-hydroxy-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

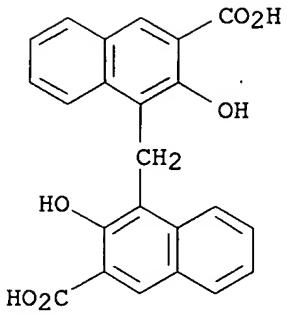
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

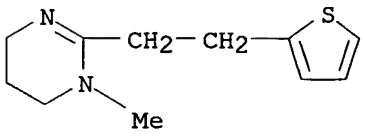
CRN 130-85-8
CMF C23 H16 O6



RN 5671-35-2 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, maleate (8CI) (CA INDEX NAME)

CM 1

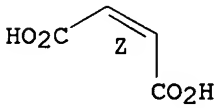
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

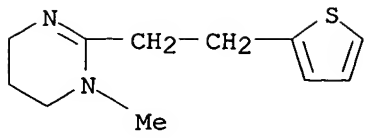
Double bond geometry as shown.



RN 5671-36-3 CAPLUS
CN Stearic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

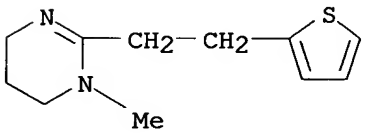
CRN 57-11-4
CMF C18 H36 O2

$HO_2C-(CH_2)_{16}-Me$

RN 5671-37-4 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2R,3R)-2,3-dihydroxybutanedioate (9CI) (CA INDEX NAME)

CM 1

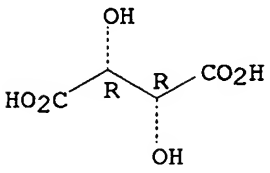
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.

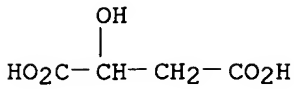


RN 5671-38-5 CAPLUS
CN Malic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

CM 1

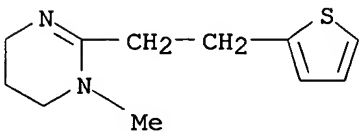
CRN 6915-15-7

CMF C4 H6 O5



CM 2

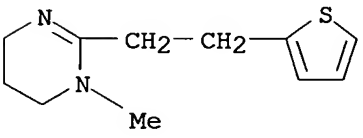
CRN 5685-90-5
CMF C11 H16 N2 S



RN 5671-39-6 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, fumarate (8CI) (CA INDEX NAME)

CM 1

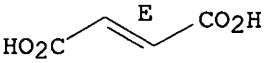
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

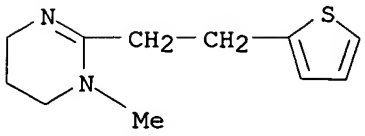


RN 5671-40-9 CAPLUS
CN Succinic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

CM 1

CRN 5685-90-5

CMF C11 H16 N2 S



CM 2

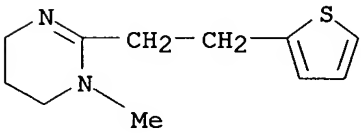
CRN 110-15-6
CMF C4 H6 O4

$HO_2C-CH_2-CH_2-CO_2H$

RN 5671-41-0 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, acetate (8CI) (CA INDEX NAME)

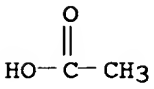
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S

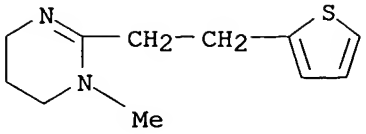


CM 2

CRN 64-19-7
CMF C2 H4 O2



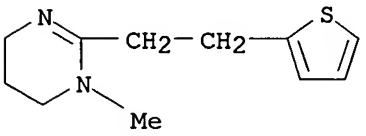
RN 5685-90-5 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]- (8CI, 9CI) (CA INDEX NAME)



RN 5707-82-4 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, oxalate (8CI) (CA INDEX NAME)

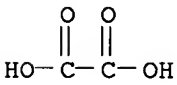
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

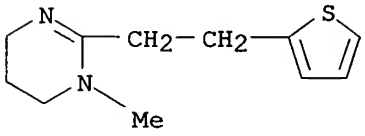
CRN 144-62-7
CMF C2 H2 O4



RN 5722-14-5 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

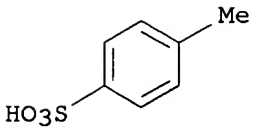
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 104-15-4

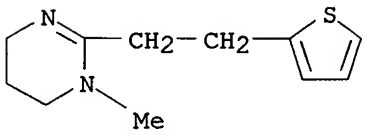
CMF C7 H8 O3 S



RN 7660-04-0 CAPLUS
CN Benzoic acid, 2-hydroxy-5-sulfo-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

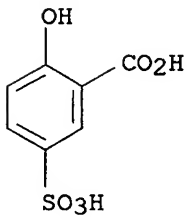
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 97-05-2
CMF C7 H6 O6 S



L17 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1962:483169 CAPLUS
DN 57:83169
OREF 57:16568b-i,16569a
TI Xanthene and thiaxanthene cyclic amidines
IN Faust, John A.; Sahyun, Melville
PA Melville Sahyun
SO 5 pp.
DT Patent
LA Unavailable

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3042674		19620703	US	19600712

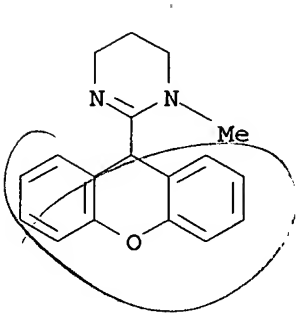
AB Xanthydrol (10 g.), 6.4 g. NCCH2CO2H, and 40 cc. AcOH was refluxed 3 hrs., cooled, poured into 500 cc. H2O, filtered, and recrystd. from dil. AcOH to give 5.7 g. 9-xanthenecyanoacetic acid (I), m. 160-3.degree.. I (5.7 g.) in 20 cc. pyridine was heated at 100-5.degree. 1.5 hrs., cooled, poured into H2O, and filtered to give crude 9-xantheneacetonitrile (II), m. 141-2.degree. (EtOH). II (2 g.) and 2 g CH2(CH2NH2)2.4MeC6H4SO3H (III) were heated at 180.degree. 2 hrs. followed by digestion with 100 cc. warm 10% HCl. The solid sepg. was 9-(1,4,5,6-tetrahydro-2-pyrimidylmethyl)xanthene HCl salt, m. 250.1.degree.. Other compds. (IV) prepd. were (starting nitrile, starting diamine monotosylate, A, R1, R2, n, % yield, and m.p. of HCl salt given): II, (CH2NH2)2 (V), O, H, 4,5-dihydro-2-imidazolyl (VI), 1, 49, 242-4.degree.; II, MeNHCH2CH2CH2NH2 (VII), O, H, 1-methyl-1,4,5,6-tetrahydro-2-pyrimidyl (VIII), 1, 22, 234-6.degree.; 10-thiaxanthylacetonitrile (IX), III, S, H, 1,4,5,6-tetrahydro-2-pyrimidyl (XI), 1, 40, 212-13.degree.; 9-xanthenecarbonitrile (XII), III, O, H, XI, 0, 23, 298-300.degree. (decompn.) [tosylate m. 275-7.degree. (decompn.)]; XII, VII, O, H, VIII, 0, 21, 250-2.degree. (decompn.); XII, V, O, H, VI, 0, 14, 280-1.degree. (decompn.) [tosylate m. 214-16.degree. (decompn.)]; 2-bromo-9-xanthylcyanide (XII), III, O, Br, XI, O, -, 317-19.degree. (decompn.); II, MeNHCH2CH2NH2, O, H, 1-methyl-4,5-dihydro-2-imidazolyl, -, -, 227-8.degree.; IX, V, S, H, VI, 1, 55, 237-8.degree. (decompn.); IX, MeCH(NH2)CH2NH2, S, H, 4-methyl-1,4,5,6-tetrahydro-2-pyrimidyl, 1, 33, 216-17.degree. (decompn.); IX, HOCH(CH2NH2)2, S, H, 5-hydroxy-1,4,5,6-tetrahydropyrimidyl, 1, 50, 279-80.degree. (decompn.); IX, III, S, H, VIII, 1, 29, 244-5.degree. (decompn.); 10-(2-chlorothiaxanthyl)acetonitrile, III, S, Cl, XI, 1, 39, 279-80.degree. (decompn.); and 10-(3-cyanopropyl)thiaxanthene (XVIII), III, S, H, XI, 3, 25, 205-6.degree.. These products displayed sedative and depressant properties. They were not toxic at 50 mg./kg. The novel starting materials used were prepd. as described below. 10-Thiaxanthenol (10.7 g.), 25.5 g. NCCH2CO2Et, 20 cc. AcOH and 50 cc. EtOH were heated on a boiling H2O bath 3 hrs., the mixt. cooled, poured into H2O, and filtered to give 14.2 g. ethyl .alpha.-cyano-.alpha.-(10-thiaxanthenyl)acetate (XIII), m. 130-1.degree. (EtOH). XIII (13.2 g.), 130 cc. 10% NaOH, and 100 cc. MeOH were stirred at 50-60.degree. 1.5 hrs. while distg. some MeOH, the mixt. dild. with H2O, acidified, and filtered to give 10.8 g. acid (XIV), m. 190-1.degree. (decompn.) (dil. EtOH). XIV (9.8 g.) and 50 cc. pyridine was refluxed 20 min., concd. to 25 cc., poured into 500 cc. H2O, triturated with dil. NaOH, and recrystd. from EtOH to give 6.3 g. IX, m. 74-5.degree.. Xanthydrol (23.0 g.), 15.0 g. KCN, and 70 cc. AcOH were shaken at 80-90.degree. in a pressure flask 24 hrs., cooled, filtered, and washed with H2O to give 15.7 g. XII, m. 99-100.degree. (EtOH). Xanthone (19.6 g.) and 62.5 g. Br was ground under H2O until most of the Br was absorbed, the solid formed washed with H2O, dried, and recrystd. from C6H6

to give 20 g. 2,7-dibromoxanthone (XV), m. 211-12.degree.. XV (30 g.) reduced with 6.9 g. Na in 37 cc. Hg in EtOH and dild. with H2O gave 13.8 g. unknown product. Further diln. gave 9 g. 2-bromo-9-xanthenol (XVI), m. 76-8.degree. (EtOH). XVI (6.8 g.), 4 g. KCN, and 50 cc. AcOH shaken in a pressure bottle at 60.degree. 12 hrs., poured into H2O, extd. with CHCl3, concd., dild. with C7H16, filtered, and the filtrate evapd. gave 5.2 g. XII, oil. To the BuLi from 1.5 g. Li in BuOH at -10.degree. was added 10 g. thiaxanthene, the mixt. refluxed under N 3 hrs., the soln. added during 15 min. under N to 60 g. CH2(CH2Br)2 in 300 cc. EtOH, stirred and refluxed 1 hr., filtered, the filtrate washed with H2O, dil. HCl, dried, and distd. gave 11 g. 10-(3-bromopropyl)thiaxanthene (XVII), b0.7 178-82.degree.. XVII (6.4 g.), 3 g. KCN, 40 cc. EtOH, and 5 cc. H2O was refluxed 7 hrs., evapd., extd. with Et2O, dried, and distd. to give 3.2 g. XVIII, b0.6 186-90.degree..

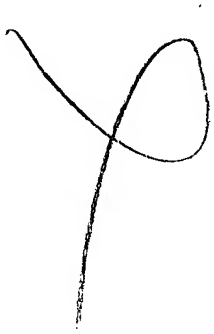
IT **98439-34-0**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-xanthen-9-yl-, hydrochloride **104099-19-6**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-(thioxanthen-9-ylmethyl)-, hydrochloride **106978-95-4**, Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-(xanthen-9-ylmethyl)-, hydrochloride
(prepn. of)

RN 98439-34-0 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-xanthen-9-yl-, hydrochloride (7CI) (CA INDEX NAME)

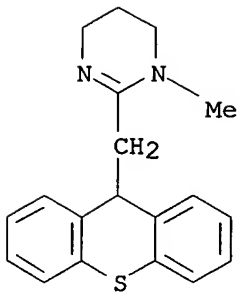


● HCl



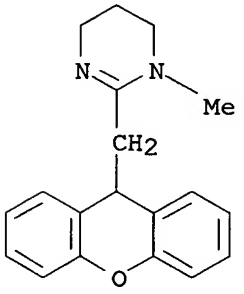
RN 104099-19-6 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-(thioxanthen-9-ylmethyl)-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 106978-95-4 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-(xanthen-9-ylmethyl)-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

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L4             QUE L3 AND L1 NOT L2
L5           0 S L4 SSS SAM
L6             SCREEN 1839
L7             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L8             STRUCTURE UPLOADED
L9             QUE L8 AND L6 NOT L7
L10         15 S L9 SSS SAM
L11            SCREEN 1839
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L18          4 L16

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L18 ANSWER 1 OF 4 CAOLD COPYRIGHT 2003 ACS on STN
AN CA64:8192c CAOLD
TI anthelmintic 2-alkylthiophenes
PA Pfizer Corp.
DT Patent

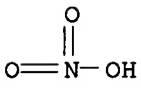
PATENT NO.	KIND	DATE
BE 658987		
GB 1045838		

IT **5671-30-7** **5671-32-9** **5671-33-0**
5671-34-1 **5671-35-2** **5671-36-3**
5671-37-4 **5671-38-5** **5671-39-6**
5671-40-9 **5671-41-0** **5671-52-3**
5685-90-5 **5707-82-4** **5722-14-5**
5822-06-0 **7660-04-0** **96773-30-7**

RN 5671-30-7 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, mononitrate (8CI, 9CI) (CA INDEX NAME)

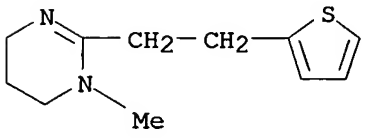
CM 1

CRN 7697-37-2
CMF H N O3



CM 2

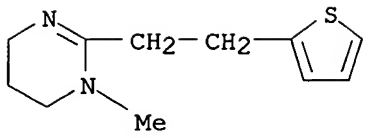
CRN 5685-90-5
CMF C11 H16 N2 S



RN 5671-32-9 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (9CI) (CA INDEX NAME)

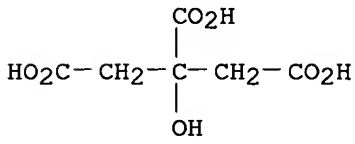
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S

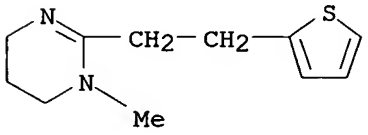


CM 2

CRN 77-92-9
CMF C6 H8 O7



RN 5671-33-0 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, monohydrochloride (8CI, 9CI) (CA INDEX NAME)

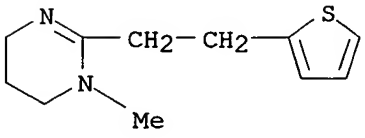


● HCl

RN 5671-34-1 CAOLD
CN 2-Naphthoic acid, 4,4'-methylenebis[3-hydroxy-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

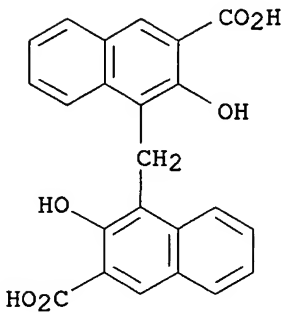
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

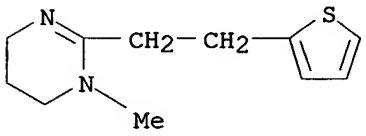
CRN 130-85-8
CMF C23 H16 O6



RN 5671-35-2 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, maleate (8CI) (CA INDEX NAME)

CM 1

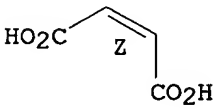
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 110-16-7
CMF C4 H4 O4

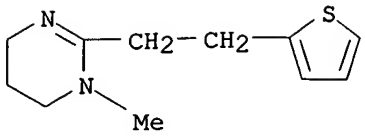
Double bond geometry as shown.



RN 5671-36-3 CAOLD
CN Stearic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

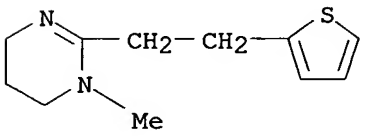
CRN 57-11-4
CMF C18 H36 O2

$HO_2C-(CH_2)_{16}-Me$

RN 5671-37-4 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, (2R,3R)-2,3-dihydroxybutanedioate (9CI) (CA INDEX NAME)

CM 1

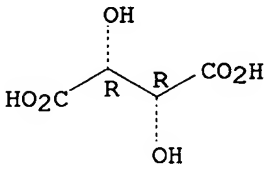
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 87-69-4
CMF C4 H6 O6

Absolute stereochemistry.

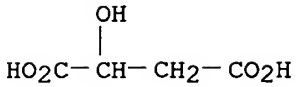


RN 5671-38-5 CAOLD
CN Malic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

CM 1

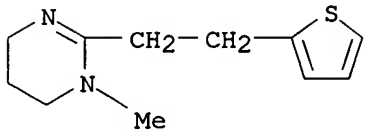
CRN 6915-15-7

CMF C4 H6 O5



CM 2

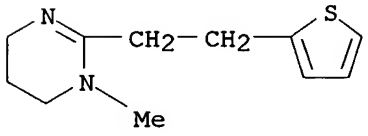
CRN 5685-90-5
CMF C11 H16 N2 S



RN 5671-39-6 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, fumarate (8CI) (CA INDEX NAME)

CM 1

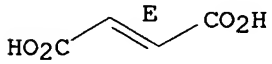
CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

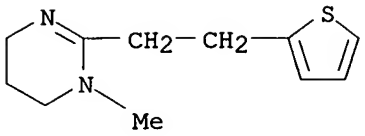


RN 5671-40-9 CAOLD
CN Succinic acid, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (8CI) (CA INDEX NAME)

CM 1

CRN 5685-90-5

CMF C11 H16 N2 S



CM 2

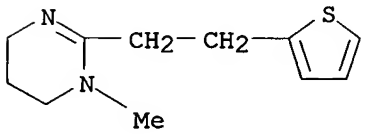
CRN 110-15-6
CMF C4 H6 O4

$HO_2C-CH_2-CH_2-CO_2H$

RN 5671-41-0 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, acetate (8CI) (CA INDEX NAME)

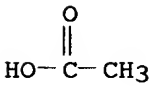
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

CRN 64-19-7
CMF C2 H4 O2

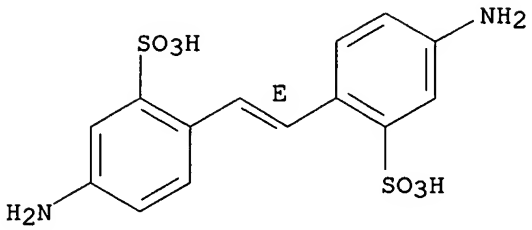


RN 5671-52-3 CAOLD
CN 2,2'-Stilbenedisulfonic acid, 4,4'-diamino-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:2), (Z)- (8CI) (CA INDEX NAME)

CM 1

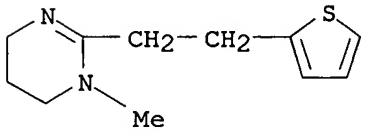
CRN 28096-93-7
CMF C14 H14 N2 O6 S2

Double bond geometry as shown.

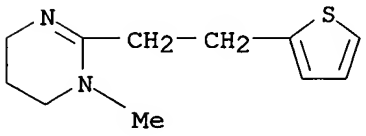


CM 2

CRN 5685-90-5
CMF C11 H16 N2 S



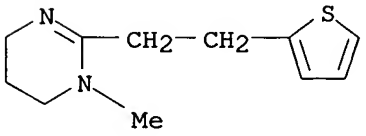
RN 5685-90-5 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]- (8CI, 9CI) (CA INDEX NAME)



RN 5707-82-4 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, oxalate (8CI) (CA INDEX NAME)

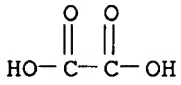
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

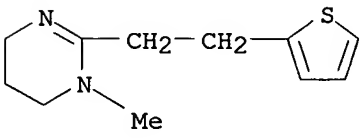
CRN 144-62-7
CMF C2 H2 O4



RN 5722-14-5 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

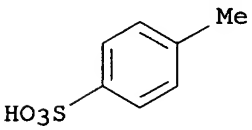
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

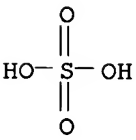
CRN 104-15-4
CMF C7 H8 O3 S



RN 5822-06-0 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]-, sulfate (1:1) (8CI, 9CI) (CA INDEX NAME)

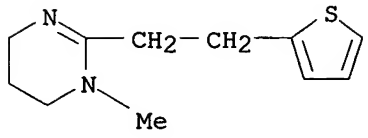
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

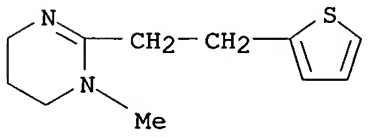
CRN 5685-90-5
CMF C11 H16 N2 S



RN 7660-04-0 CAOLD
CN Benzoic acid, 2-hydroxy-5-sulfo-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

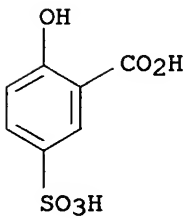
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

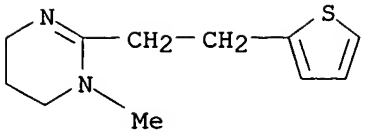
CRN 97-05-2
CMF C7 H6 O6 S



RN 96773-30-7 CAOLD
CN 2,2'-Stilbenedisulfonic acid, 4,4'-diamino-, compd. with 1,4,5,6-tetrahydro-1-methyl-2-[2-(2-thienyl)ethyl]pyrimidine (7CI) (CA INDEX NAME)

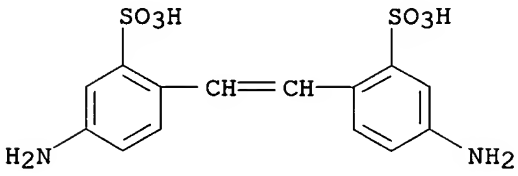
CM 1

CRN 5685-90-5
CMF C11 H16 N2 S



CM 2

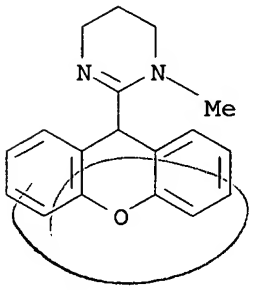
CRN 81-11-8
CMF C14 H14 N2 O6 S2



L18 ANSWER 2 OF 4 CAOLD COPYRIGHT 2003 ACS on STN
AN CA57:16568b CAOLD
TI xanthene and thiaxanthene cyclic amidines
AU Faust, John A.; Sahyun, M.
DT Patent
TI xanthene and thiaxanthene cyclic amidines
AU Sahyun, Melville
DT Patent

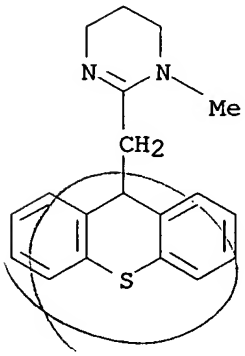
PATENT NO.	KIND	DATE
US 3042674		1962

IT **98439-34-0 104099-19-6 106978-95-4**
RN 98439-34-0 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-xanthen-9-yl-, hydrochloride (7CI) (CA INDEX NAME)



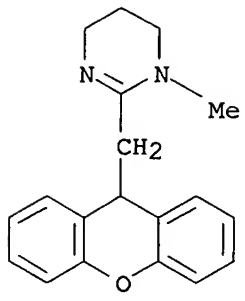
● HCl

RN 104099-19-6 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-(thioxanthen-9-ylmethyl)-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 106978-95-4 CAOLD
CN Pyrimidine, 1,4,5,6-tetrahydro-1-methyl-2-(xanthen-9-ylmethyl)-, hydrochloride (7CI) (CA INDEX NAME)

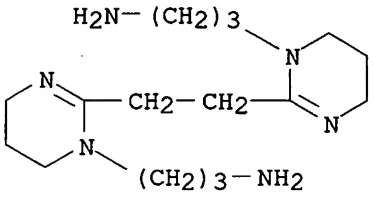


● HCl

L18 ANSWER 3 OF 4 CAOLD COPYRIGHT 2003 ACS on STN
AN CA53:5665d CAOLD
TI hydrocarbon distillates, stabilization of
PA Universal Oil Products Co.
DT Patent
TI stabilization of hydrocarbon distillates
AU Cyba, Henry A.; Thompson, R. B.
DT Patent

PATENT NO.	KIND	DATE
US 2844446		1958

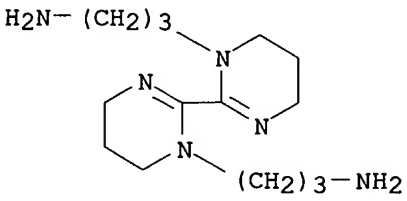
IT **107154-73-4**
RN 107154-73-4 CAOLD
CN Pyrimidine, 2,2'-ethylenebis[1-(3-aminopropyl)-1,4,5,6-tetrahydro- (6CI) (CA INDEX NAME)



Gave on #37

L18 ANSWER 4 OF 4 CAOLD COPYRIGHT 2003 ACS on STN
AN CA52:3690c CAOLD
TI reaction of cyanogen with org. compds. - (X) aliphatic and aromatic diamines
AU Woodburn, Henry M.; Fisher, J. R.
IT **106522-59-2**
RN 106522-59-2 CAOLD
CN 2,2'-Bipyrimidine, 1,1'-bis(3-aminopropyl)-1,1',4,4',5,5',6,6'-octahydro-(6CI) (CA INDEX NAME)

Same #3



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=> log y
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              10.88     338.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00     -25.39

STN INTERNATIONAL LOGOFF AT 21:24:36 ON 13 DEC 2003
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